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LOGINID:ssptajem1625

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	MAY 01	New CAS web site launched
NEWS 3	MAY 08	CA/CAplus Indian patent publication number format defined
NEWS 4	MAY 14	RDISCLOSURE on STN Easy enhanced with new search and display fields
NEWS 5	MAY 21	BIOSIS reloaded and enhanced with archival data
NEWS 6	MAY 21	TOXCENTER enhanced with BIOSIS reload
NEWS 7	MAY 21	CA/CAplus enhanced with additional kind codes for German patents
NEWS 8	MAY 22	CA/CAplus enhanced with IPC reclassification in Japanese patents
NEWS 9	JUN 27	CA/CAplus enhanced with pre-1967 CAS Registry Numbers
NEWS 10	JUN 29	STN Viewer now available
NEWS 11	JUN 29	STN Express, Version 8.2, now available
NEWS 12	JUL 02	LEMBASE coverage updated
NEWS 13	JUL 02	LMEDLINE coverage updated
NEWS 14	JUL 02	SCISEARCH enhanced with complete author names
NEWS 15	JUL 02	CHEMCATS accession numbers revised
NEWS 16	JUL 02	CA/CAplus enhanced with utility model patents from China
NEWS 17	JUL 16	CAplus enhanced with French and German abstracts
NEWS 18	JUL 18	CA/CAplus patent coverage enhanced
NEWS 19	JUL 26	USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS 20	JUL 30	USGENE now available on STN
NEWS 21	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS 22	AUG 06	BEILSTEIN updated with new compounds
NEWS 23	AUG 06	FSTA enhanced with new thesaurus edition

NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:26:13 ON 06 AUG 2007

=> file reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 14:26:41 ON 06 AUG 2007

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 5 AUG 2007 HIGHEST RN 944042-79-9
DICTIONARY FILE UPDATES: 5 AUG 2007 HIGHEST RN 944042-79-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

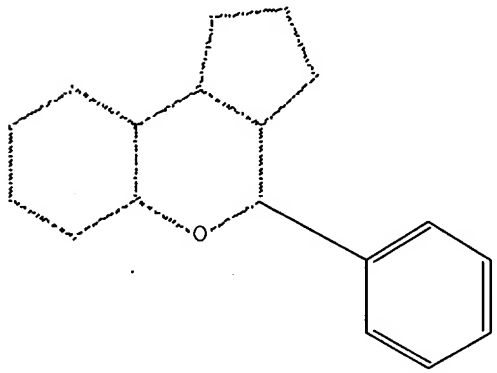
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10-552504.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam
SAMPLE SEARCH INITIATED 14:28:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1636 TO ITERATE

100.0% PROCESSED 1636 ITERATIONS 17 ANSWERS
SEARCH TIME: 00.00.01

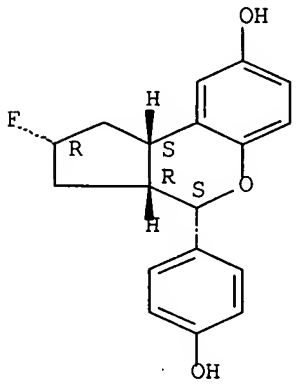
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 30294 TO 35146
PROJECTED ANSWERS: 93 TO 587

L2 17 SEA SSS SAM L1

=> d scan

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Cyclopenta[c][1]benzopyran-8-ol, 2-fluoro-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (2R,3aR,4S,9bS)- (9CI)
MF C18 H17 F O3

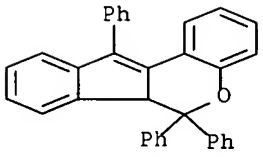
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

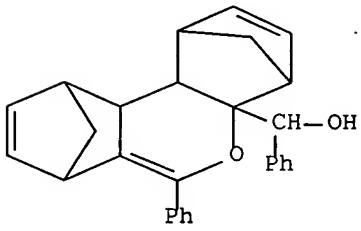
L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11-triphenyl- (4CI)
MF C34 H24 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 1,4:7,10-Dimethano-4aH-dibenzo[b,d]pyran-4a-methanol, 1,4,7,10,10a,10b-hexahydro-α,6-diphenyl-, [1α,4α,4aβ(R*),7β,10.beta.,10aα,10bβ]- (9CI)
MF C28 H26 O2

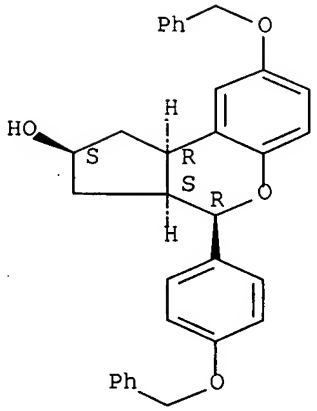


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Cyclopenta[c][1]benzopyran-2-ol, 1,2,3,3a,4,9b-hexahydro-8-(phenylmethoxy)-4-[4-(phenylmethoxy)phenyl]-, (2R,3aR,4S,9bS)-rel- (9CI)
MF C32 H30 O4

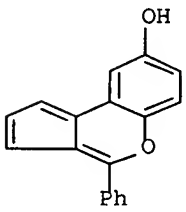
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

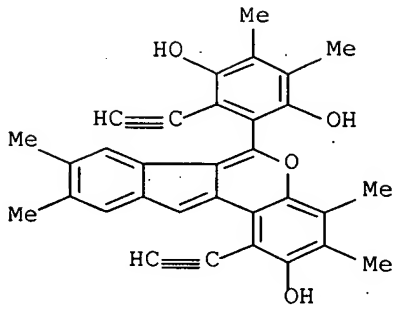
L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Cyclopenta[c][1]benzopyran-8-ol, 4-phenyl- (9CI)
MF C18 H12 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 1,4-Benzenediol, 2-ethynyl-3-(1-ethynyl-2-hydroxy-3,4,8,9-tetramethylbenz[b]indeno[2,1-d]pyran-6-yl)-5,6-dimethyl- (9CI)
MF C32 H26 O4

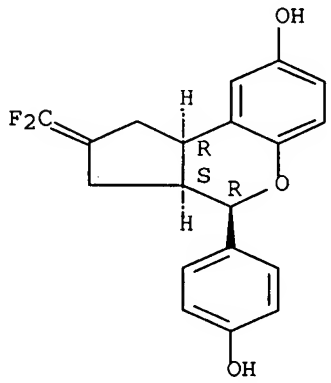


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Cyclopenta[c][1]benzopyran-8-ol, 2-(difluoromethylene)-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aS,4R,9bR)- (9CI)
MF C19 H16 F2 O3

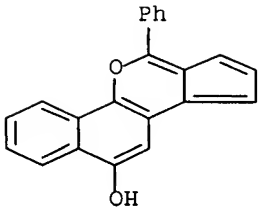
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

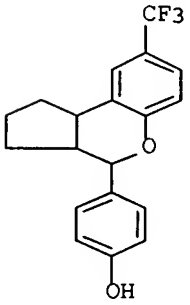
L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Cyclopenta[d]naphtho[1,2-b]pyran-11-ol, 6-phenyl- (9CI)
MF C22 H14 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Phenol, 4-[1,2,3,3a,4,9b-hexahydro-8-(trifluoromethyl)cyclopenta[c][1]benzopyran-4-yl]- (9CI)
MF C19 H17 F3 O2



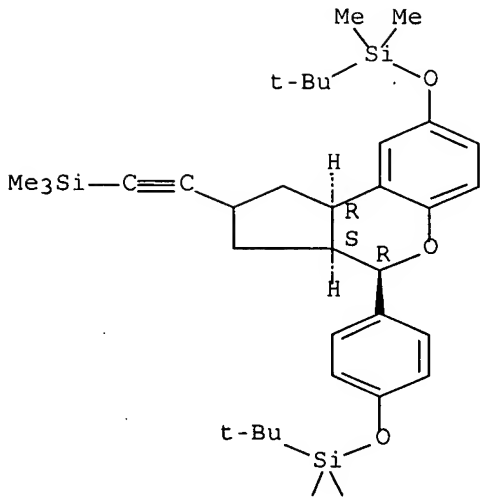
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Silane, (1,1-dimethylethyl)[4-[(3aR,4S,9bS)-8-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1,2,3,3a,4,9b-hexahydro-2-[(trimethylsilyl)ethynyl]cyclopenta[c][1]benzopyran-4-yl]phenoxy]dimethyl-, rel- (9CI)
MF C35 H54 O3 Si3

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

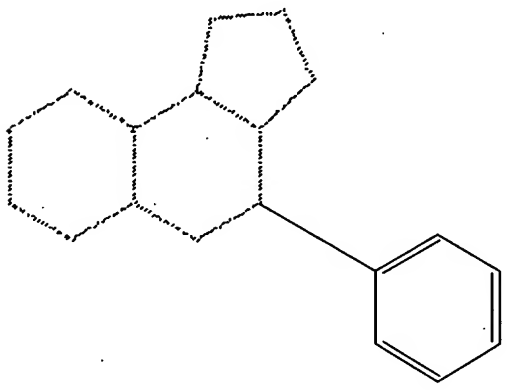
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=>
Uploading C:\Program Files\Stnexp\Queries\10-552504a.str

L3 STRUCTURE UPLOADED

=> d l3
L3 HAS NO ANSWERS
L3 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l3 sss sam
SAMPLE SEARCH INITIATED 14:43:40 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2835 TO ITERATE

70.5% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 53507 TO 59893
PROJECTED ANSWERS: 0 TO 0

L4 0 SEA SSS SAM L3

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 13.95 14.16

FILE 'CAPLUS' ENTERED AT 14:45:00 ON 06 AUG 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 6 Aug 2007 VOL 147 ISS 7
FILE LAST UPDATED: 5 Aug 2007 (20070805/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l2 and (py<2004 or ay<2004 or pry<2004)
8 L2
23927525 PY<2004
4731037 AY<2004
4212934 PRY<2004
L5 6 L2 AND (PY<2004 OR AY<2004 OR PRY<2004)

=> d scan

L5 6 ANSWERS CAPLUS COPYRIGHT 2007 ACS on STN
IC ICM C07D311-00

CC 27-7 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 63

TI Preparation of substituted benzopyrans as selective estrogen receptor-beta agonists

ST benzopyran prepn estrogen receptor beta agonist anticancer

IT Prostate gland, disease
(benign hyperplasia; preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

IT Hyperplasia
(benign prostatic; preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

IT Human
Prostate gland, neoplasm
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

IT Antitumor agents
(prostate gland; preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

IT Estrogen receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(β; preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

IT **787621-59-4P** **787621-60-7P** **787621-80-1P** **787621-81-2P**
787622-06-4P **787622-10-0P** **787622-73-5P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

IT **787621-53-8P** **787621-54-9P** **787621-55-0P** **787621-56-1P** **787621-57-2P**
787621-58-3P **787621-61-8P** **787621-62-9P** **787621-63-0P** **787621-64-1P**
787621-69-6P **787621-72-1P** **787621-73-2P** **787621-75-4P** **787621-77-6P**
787621-78-7P **787621-82-3P** **787621-83-4P** **787621-85-6P** **787621-86-7P**
787621-88-9P **787621-90-3P** **787621-91-4P** **787621-93-6P**
787621-94-7P **787621-96-9P** **787621-97-0P** **787621-98-1P**
787621-99-2P **787622-11-1P** **787622-13-3P** **787622-22-4P**
787622-31-5P **787622-32-6P** **787622-33-7P** **787622-34-8P** **787622-36-0P**
787622-37-1P **787622-39-3P** **787622-40-6P** **787622-42-8P**
787622-43-9P **787622-44-0P** **787622-49-5P** **787622-50-8P**
787622-51-9P **787622-52-0P** **787622-54-2P** **787622-55-3P** **787622-56-4P**
787622-57-5P **787622-58-6P** **787622-59-7P** **787622-68-8P** **787622-69-9P**
787622-70-2P **787622-71-3P** **787622-72-4P** **787622-74-6P** **787622-75-7P**
787622-76-8P **787622-77-9P** **787622-78-0P** **787622-79-1P**
787622-80-4P **787622-81-5P** **787622-82-6P** **787622-83-7P** **787622-84-8P**
787622-85-9P **787622-86-0P** **787622-87-1P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

IT 62-23-7, p-Nitrobenzoic acid 75-86-5, Acetone cyanohydrin 96-33-3, Methyl acrylate 96-35-5, Methyl glycolate 100-39-0, Benzyl bromide 123-31-9, Hydroquinone, reactions 623-82-5, (R)-(+)-3-Methyladipic acid 892-20-6, Triphenyltin hydride 1066-54-2, Trimethylsilylacetylene 1100-88-5, Benzyltriphenylphosphonium chloride 1530-32-1, Ethyltriphenylphosphonium bromide 2365-48-2, Methyl thioglycolate 2622-05-1, Allylmagnesium chloride 3058-01-3, 3-Methyladipic acid 5781-53-3, Methyl chloroglyoxylate 6228-47-3, Propyltriphenylphosphonium bromide 6793-92-6, p-Benzyloxybromobenzene 10347-88-3, 3-tert-Butyladipic acid 10538-51-9, 2,5-Dimethoxycinnamic acid

22444-89-9, Butyltriphenylphosphonium 25458-45-1, 1-Bromo-4-(methoxymethoxy)benzene 37595-74-7, N-Phenyltrifluoromethanesulfonimide 38053-91-7, 2-[(Trimethylsilyl)oxy]butadiene 38078-09-0, N,N-Diethylaminosulfur trifluoride 70160-51-9 72047-94-0, [2-(Acetoxymethyl)allyl]trimethylsilane 108270-19-5 146631-00-7, 4-(Benzyloxy)phenylboronic acid 787622-05-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

IT 2689-68-1P 4463-74-5P 6093-68-1P, 6-Hydroxycoumarin 57595-23-0P 87905-74-6P, 1,4-Bis(methoxymethoxy)benzene 608536-53-4P, 6-Methoxymethoxycoumarin 787621-46-9P 787621-47-0P 787621-48-1P 787621-49-2P 787621-50-5P 787621-51-6P 787621-52-7P 787621-65-2P 787621-66-3P 787621-67-4P 787621-68-5P 787621-70-9P 787621-71-0P 787621-74-3P 787621-76-5P 787621-79-8P 787621-84-5P 787621-87-8P 787621-89-0P 787621-92-5P 787621-95-8P 787622-00-8P 787622-01-9P 787622-02-0P 787622-03-1P 787622-04-2P 787622-07-5P 787622-08-6P 787622-09-7P 787622-12-2P 787622-14-4P 787622-15-5P 787622-16-6P 787622-18-8P 787622-19-9P 787622-20-2P 787622-21-3P 787622-23-5P, 6-Benzyloxychromen-2-one 787622-25-7P 787622-26-8P 787622-27-9P 787622-28-0P **787622-29-1P** 787622-30-4P 787622-35-9P 787622-38-2P **787622-41-7P** 787622-45-1P 787622-46-2P 787622-47-3P 787622-48-4P 787622-60-0P 787622-61-1P 787622-62-2P 787622-63-3P 787622-64-4P 787622-65-5P 787622-66-6P 787622-67-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L5 6 ANSWERS CAPLUS COPYRIGHT 2007 ACS on STN
CC 10 (Organic Chemistry)
TI Condensation of tetraphenylbutynediol with phenol
IT Catalysts
(for condensation, of PhOH with 1,1,4,4-tetraphenyl-2-butyne-1,4-diol)
IT 411220-98-9P, Indene, 1-benzohydrylidene-2-chloro-3-phenyl- 411220-98-9P, Methane, (2-chloro-3-phenyl-1-indenylidene)diphenyl- 854748-48-4P, Methane, [2-(p-methoxyphenyl)-3-phenyl-1-indenylidene]diphenyl- 854748-48-4P, Anisole, p-(1-benzohydrylidene-3-phenyl-2-indenyl)- 854748-48-4P, Indene, 1-benzohydrylidene-2-(p-methoxyphenyl)-3-phenyl- 854749-76-1P, Indene, 1-benzohydrylidene-2-phenoxy-3-phenyl- 854749-76-1P, Methane, (2-phenoxy-3-phenyl-1-indenylidene)diphenyl- 860000-10-8P, Furan, 2,5-dihydro-3-phenoxy-2,2,5,5-tetraphenyl- **860186-11-4P**, Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11-triphenyl- 861008-63-1P, Phenol, p-(1-benzohydrylidene-3-phenyl-2-indenyl)-
RL: PREP (Preparation)
(preparation of)
IT 1483-74-5, 2-Butyne-1,4-diol, tetraphenyl-
(reaction with phenol)
IT 108-95-2, Phenol
(reactions of, with 1,1,4,4-tetraphenyl-2-butyne-1,4-diol)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

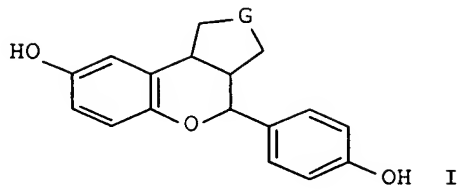
=> d ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 6 ANSWERS - CONTINUE? Y/(N):y

L5 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:927190 CAPLUS Full-text
DOCUMENT NUMBER: 141:395410
TITLE: Preparation of substituted benzopyrans as selective estrogen receptor-beta agonists
INVENTOR(S): Durst, Gregory Lee; Norman, Bryan Hurst; Pfeifer, Lance Allen; Richardson, Timothy Ivo
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 129 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2004094400	A2	20041104	WO 2004-US9272		20040408 <--
WO 2004094400	A3	20050224			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 2004232798	A1	20041104	AU 2004-232798		20040408 <--
CA 2518819	A1	20041104	CA 2004-2518819		20040408 <--
EP 1626974	A2	20060222	EP 2004-759767		20040408 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK					
BR 2004009588	A	20060418	BR 2004-9588		20040408 <--
CN 1777614	A	20060524	CN 2004-80010817		20040408 <--
JP 2006524240	T	20061026	JP 2006-509332		20040408 <--
US 2007106082	A1	20070510	US 2005-552504		20051006 <--
MX 2005PA11243	A	20051215	MX 2005-PA11243		20051019 <--
PRIORITY APPLN. INFO.:			US 2003-464404P	P	20030421 <--
			WO 2004-US9272	W	20040408

OTHER SOURCE(S): MARPAT 141:395410
GI



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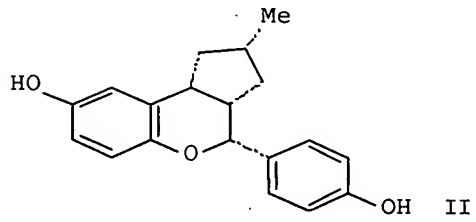


II

AB Title compds. represented by the formula I [wherein G = CH-alkyl, CO, CHOH, CHCF3, CF2, C(OH)CF3, CH(OH)alkyl, CH-O-alkyl, CHOCO-alkyl, etc; and their enantiomers, and pharmaceutically acceptable salts thereof] were prepared as estrogen receptor (ER)-beta agonists. For example, II was given in a multi-step synthesis starting from hydroquinone. I exhibited binding affinities (Kis) at the ER-α subtype in the range 5.0 - >10,000 nM and to the ER-β subtype in the range of 0.20 - 429 nM. Thus, I and their pharmaceutical compns. are useful as estrogen receptor agonists for the treatment of estrogen receptor mediated diseases such as prostate cancer or benign prostate hyperplasia.

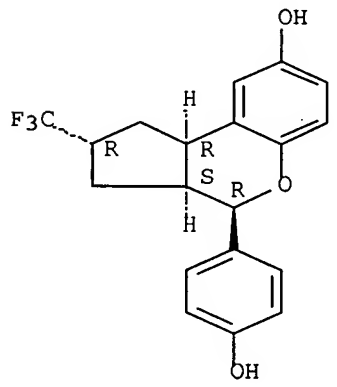
IT **787621-81-2P**

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

RN 787621-81-2 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-(trifluoromethyl)-, (2R,3aS,4R,9bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

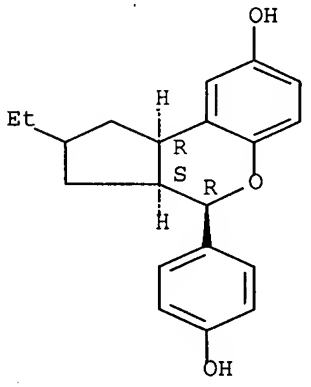


IT **787621-88-9P 787621-99-2P 787622-40-6P**
787622-43-9P 787622-78-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

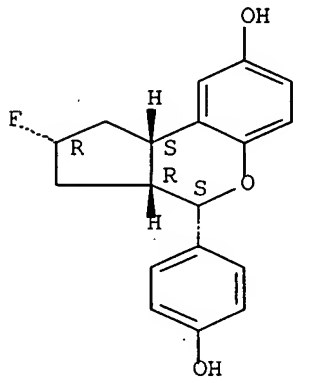
RN 787621-88-9 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 2-ethyl-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



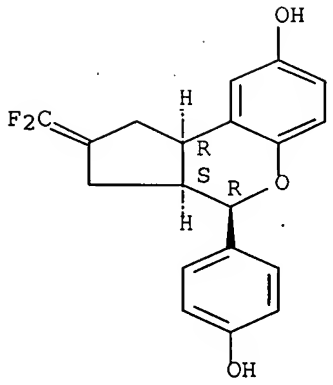
RN 787621-99-2 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 2-fluoro-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (2R,3aR,4S,9bS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



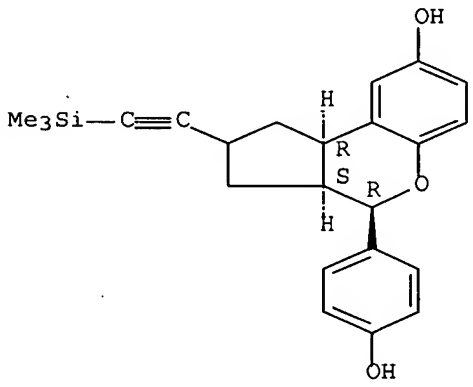
RN 787622-40-6 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 2-(difluoromethylene)-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aS,4R,9bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



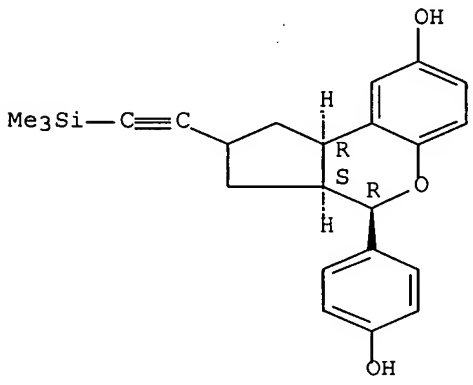
RN 787622-43-9 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-[(trimethylsilyl)ethynyl]-, (3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 787622-78-0 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-[(trimethylsilyl)ethynyl]-, (3aS,4R,9bR)- (9CI) (CA INDEX NAME)

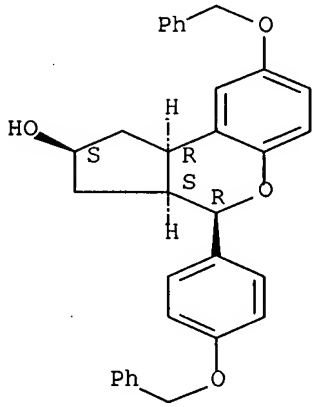
Absolute stereochemistry.



IT **787622-29-1P 787622-41-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

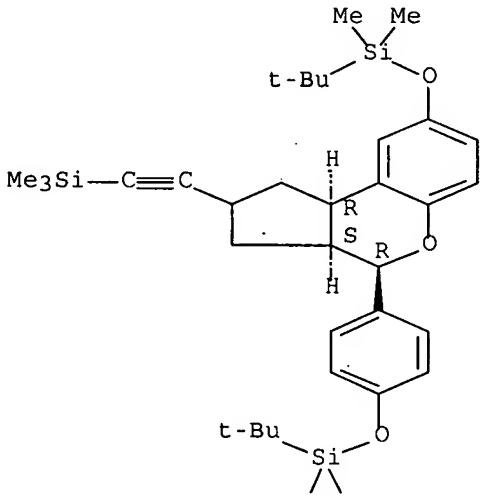
RN 787622-29-1 CAPLUS
CN Cyclopenta[c][1]benzopyran-2-ol, 1,2,3,3a,4,9b-hexahydro-8-(phenylmethoxy)-4-[4-(phenylmethoxy)phenyl]-, (2R,3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 787622-41-7 CAPLUS
CN Silane, (1,1-dimethylethyl)[4-[(3aR,4S,9bS)-8-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1,2,3,3a,4,9b-hexahydro-2-[(trimethylsilyl)ethynyl]cyclopenta[c][1]benzopyran-4-yl]phenoxy]dimethyl-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



Me Me

L5 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:417738 CAPLUS Full-text
DOCUMENT NUMBER: 139:6768
TITLE: Preparation of benzopyran derivatives as selective estrogen receptor β agonists
INVENTOR(S): Dodge, Jeffrey Alan; Krishnan, Venkatesh Gary; Lugar, Charles Willis, III; Neubauer, Blake Lee; Norman, Bryan Hurst; Pfeifer, Lance Allen; Richardson, Timothy Ivo
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 138 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003044006	A1	20030530	WO 2002-US33622	20021107 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2467013	A1	20030530	CA 2002-2467013	20021107 <--
AU 2002359283	A1	20030610	AU 2002-359283	20021107 <--
EP 1448544	A1	20040825	EP 2002-793806	20021107 <--
EP 1448544	B1	20070516		
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CN 1589268	A	20050302	CN 2002-822991	20021107 <--
HU 200402628	A2	20050428	HU 2004-2628	20021107 <--
JP 2005513027	T	20050512	JP 2003-545643	20021107 <--
NZ 531850	A	20070126	NZ 2002-531850	20021107 <--
EP 1790644	A1	20070530	EP 2007-102693	20021107 <--
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AT 362471	T	20070615	AT 2002-793806	20021107 <--
US 2004249167	A1	20041209	US 2004-493092	20040420 <--
US 7217734	B2	20070515		
ZA 2004003733	A	20051004	ZA 2004-3733	20040514 <--
IN 2004KN00639	A	20060421	IN 2004-KN639	20040517 <--
MX 2004PA04703	A	20040819	MX 2004-PA4703	20040518 <--
NO 2004002583	A	20040618	NO 2004-2583	20040618 <--
PRIORITY APPLN. INFO.:			US 2001-332766P P	20011119 <--
			US 2002-363622P P	20020311 <--
			EP 2002-793806 A3	20021107 <--

WO 2002-US33622 W 20021107 <--

OTHER SOURCE(S): MARPAT 139:6768

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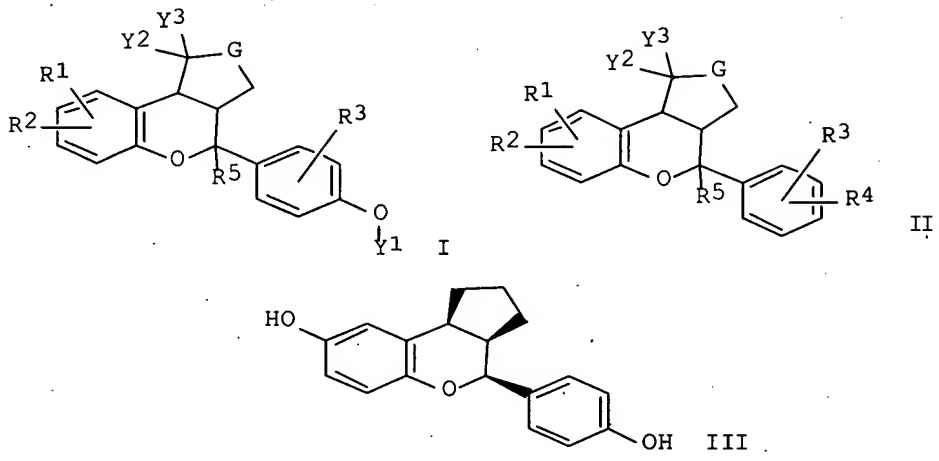


I II

III

AB The title compds. I and II [wherein R1-R4 = independently H, alkyl, OH, alkoxy, halo, amido, or CF3; R5 = H or CF3; Y1-Y3 = independently H or alkyl; G = CH2, CH2CH2, or CH2CH2CH2] and stereoisomers, and pharmaceutical acceptable salts thereof are prepared as selective estrogen receptor β agonists for the treatment of prostate cancer. For example, the benzopyran III was prepared in a multi-step synthesis in moderate yield. III binds to estrogen receptor β (ER β) with a Ki of <1 nM and Ki(ER α)/Ki(ER β) of 8.0.

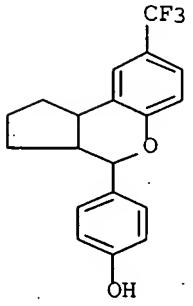
IT **533884-11-6P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of benzopyran derivs. as selective estrogen receptor β agonists)

RN 533884-11-6 CAPLUS

CN Phenol, 4-[1,2,3,3a,4,9b-hexahydro-8-(trifluoromethyl)cyclopenta[c][1]benzopyran-4-yl]- (9CI) (CA INDEX NAME)

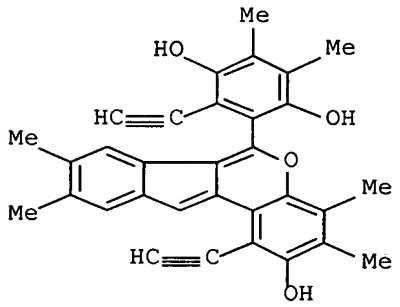


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:689997 CAPLUS Full-text
DOCUMENT NUMBER: 130:38272
TITLE: A novel tandem bicyclization to form an indenopyran ring system
AUTHOR(S): Chakraborty, Manisha; McConville, David B.; Saito, Takeshi; Meng, Huihan; Rinaldi, Peter L.; Tessier, Claire A.; Youngs, Wiley J.
CORPORATE SOURCE: Dep. of Chemistry, University of Akron, Akron, OH, 44325-3601, USA
SOURCE: Tetrahedron Letters (1998), 39(45), 8237-8340
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:38272

AB A new palladium-copper catalyzed intramol. acetylene-zipper type bicyclization between alkyne and hydroxy functionality of an alkynyl hydroquinone has been observed to give a highly conjugated ring system.

IT **216777-12-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of indenopyrans by tandem bicyclization)
RN 216777-12-7 CAPLUS
CN 1,4-Benzenediol, 2-ethynyl-3-(1-ethynyl-2-hydroxy-3,4,8,9-tetramethylbenz[b]indeno[2,1-d]pyran-6-yl)-5,6-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

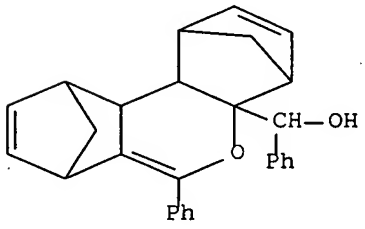
L5 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1972:152831 CAPLUS Full-text
DOCUMENT NUMBER: 76:152831
TITLE: Condensation of phenyl ethynyl ketone with cyclopentadiene. Reinvestigation
AUTHOR(S): Venkataramani, P. S.; Chandrasekharan, S.; Swaminathan, S.
CORPORATE SOURCE: Dep. Org. Chem., Univ. Madras, Madras, India
SOURCE: Tetrahedron (1972), 28(5), 1249-55
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.

AB The earlier structural assignment of 2-benzoylnorborna-diene (I) for the product obtained by the condensation of PhC-(O)C.tplbond.CH with cyclopentadiene is now revised to a dimeric structure, II.

IT **36144-49-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 36144-49-7 CAPLUS

CN 1,4:7,10-Dimethano-4aH-dibenzo[b,d]pyran-4a-methanol, 1,4,7,10,10a,10b-hexahydro-α,6-diphenyl-, [1α,4α,4aβ(R*),7β,10.beta.,10aα,10bβ]- (9CI) (CA INDEX NAME)



L5 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1969:77707 CAPLUS Full-text

DOCUMENT NUMBER: 70:77707

TITLE: Experiments in the brazilane series. I. Preparation of 2-phenyl-5',6',7-trimethoxybrazilane

AUTHOR(S): Morsingh, Francis

CORPORATE SOURCE: Univ. Malaya, Kuala Lumpur, Malay.

SOURCE: Tetrahedron (1969), 25(2), 355-9
CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

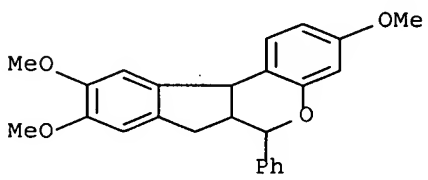
LANGUAGE: English

AB Superposition of flavan on brazilane would afford 2-phenylbrazilane. Although this structure has not yet been isolated, biogenetically it is feasible. The synthesis of 2-phenyl-5',6',7-trimethoxybrazilane is described.

IT **21834-73-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 21834-73-1 CAPLUS

CN Benz[b]indeno[1,2-d]pyran, 6,6a,7,11b-tetrahydro-3,9,10-trimethoxy-6-phenyl- (8CI) (CA INDEX NAME)



L5 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1946:23981 CAPLUS Full-text

DOCUMENT NUMBER: 40:23981

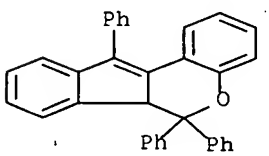
ORIGINAL REFERENCE NO.: 40:4709e-i,4710a-b
TITLE: Condensation of tetraphenylbutynediol with phenol
AUTHOR(S): Zal'kind, Yu. S.; Teterin, V. K.; Kuznetsov, S. G.
CORPORATE SOURCE: Leningrad Chem. Tech. Inst.
SOURCE: Zhurnal Obshchei Khimii (1945), 15, 488-98
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB [.tplbond.CC(OH)Ph2]2 (I) (30 g.), 87.6 g. PhOH, 60 cc. benzene and 0.4 g. dry H2NC6H4SO3H were refluxed for 2 h. with continuous removal of water by means of a Stark-Dean type collector, in which 3.35 cc. H2O was collected at the end of the reaction; after cooling and dilution with benzene, the crystalline and the liquid portions were steam-distilled to remove the solvent. There were obtained 28.7 g. crystalline matter and 16.7 g. red resin. Prolonged recrystn. from benzene, CHCl3, and ligroin gave the following products: 21.5 g. 1-diphenylmethylene-2-p-hydroxyphenyl-3-phenylindene, m. 255° (II), yellow-orange needles; 2.8 g. 1-diphenylmethylene-2- phenoxy-3-phenylindene (III), m. 223°, orange prisms; 1.2 g. 2,2,5,5-tetraphenyl-3-phenoxy-2,5-dihydrofuran, m. 176°, colorless needles; and 0.4 g. 2,2,3'-triphenyl-1',2',3,4-indenochroman (IV), m. 216-17°, colorless parallelopipeds. II was converted into the MeO derivative, m. 176-7 °, by boiling with MeI in the presence of K2CO3 in Me2CO, or by treatment with Me2SO4 in 20% NaOH; rapid crystallization from Me2CO leads to yellow needles of the above m.p., slow crystallization gives large red-brown parallelopipeds, m. 167-8°. III was prepared by an alternate method for identification: 10.5 g. I in 150 cc. Et2O was treated with 22.5 g. PCl3 at 1°over 5 h., stirred for 2 h. at 0° and for 4 h. at room temperature to yield, after removal of the solvent, hydrolysis, and crystallization from ligroin 1.0 g. 1-diphenylmethylene-2-chloro-3- phenylindene, m. 157° (cf. Wieland and Kloss, C.A. 23, 3696), and 3 unidentified products m. 147-8° (4.5 g.), m. 194-5° (0.2 g.), and m. 165° (0.4 g.); 0.4 g. of the chloride was added to a solution of 0.1 g. K in 2 g. molten PhOH and heated slowly to 220° for 1 h.; after treatment with alkaline water, extraction of the precipitate with EtOH, and crystallization of the residue from benzene-petr. ether there was obtained a product identical with III, m. 223°, above. Boiling of this in MePh in the presence of sulfanilic acid failed to effect any isomerization. IV on boiling with alc. KOH is transformed into 2 substances which were unidentified: colorless, m. 230° (from EtOH, then EtOHMe2CO), and orange, m. 208-19°, with the former transforming into a product m. 208-14°, on heating above the m.p. The condensation of I with PhOH was also conducted in the presence of the following catalysts: activated Chasoviarskii clay, H2SO4-AcOH, and glacial AcOH. The 1st catalyst gave results similar to sulfanilic acid while the 2nd catalyst gave only II, m. 255°, in 98% yield (crude); the 3rd catalyst gave only a resinous, ill-defined mixture of some transformation products of the glycol without condensation with PhOH.

IT **860186-11-4P**, Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11-triphenyl-
RL: PREP (Preparation)
(preparation of)

RN 860186-11-4 CAPLUS

CN Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11-triphenyl- (4CI) (CA INDEX NAME)



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=> s l2 sss full
L6            8 L2

=> d ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 8 ANSWERS - CONTINUE? Y/(N):y

L6   ANSWER 1 OF 8  CAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2006:381028  CAPLUS Full-text
DOCUMENT NUMBER:          144:432681
TITLE:                    Preparation of substituted benzopyrans as selective
                          estrogen receptor-beta agonists
INVENTOR(S):              Norman, Bryan Hurst; Richardson, Timothy Ivo
PATENT ASSIGNEE(S):       Eli Lilly and Company, USA
SOURCE:                   PCT Int. Appl., 50 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.          DATE
     ---------------      ----   --------    --------------------     --------
     WO 2006044176         A1    20060427    WO 2005-US35472          20051005
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
             LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ,
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             SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN,
             YU, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
     CA 2578300            A1    20060427    CA 2005-2578300          20051005
     EP 1805160            A1    20070711    EP 2005-807448           20051005
         R:  AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR
PRIORITY APPLN. INFO.:                          US 2004-619627P     P  20041018
                                                WO 2005-US35472     W  20051005
OTHER SOURCE(S):          MARPAT 144:432681
GI
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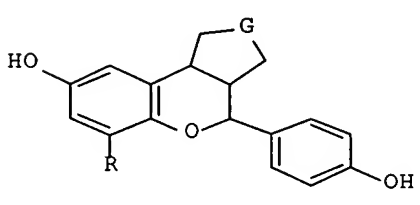

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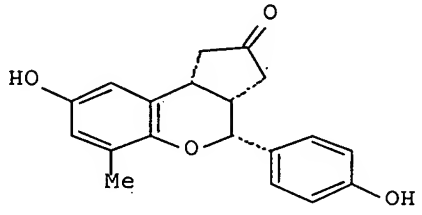


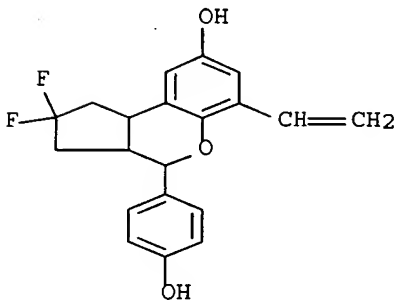
II

AB Title compds. represented by the formula I [wherein R = halo, alkyl or R3-(CH2)m; G = O, CF2, SOn, CO, CR1H or CR2(OH); R1 = F, OH, cyano, etc.; R2 = CF3 or alkyl; R3 = CN, OH, alkenyl or alkoxy(carbonyl); m = 0-2; n = 0-2; and pharmaceutical acceptable salts thereof] were prepared as estrogen receptor-beta (ER-β) agonists. For example, II was given in a multi-step synthesis starting from 3-bromo-2-hydroxy-5- methoxybenzaldehyde. I exhibited binding affinities (Kis) at the ER-α subtype in the range 4- >1000 nM and to the ER-β subtype in the range of 0.3-120 nM. Thus, I and their pharmaceutical compns. are useful as estrogen receptor agonists for the treatment of ER-β mediated diseases, such as prostate cancer or benign prostate hyperplasia (no data).

IT **885025-43-4P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted benzopyrans as selective estrogen receptor-beta agonists)

RN 885025-43-4 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 6-ethenyl-2,2-difluoro-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:369613 CAPLUS Full-text

DOCUMENT NUMBER: 144:150207

TITLE: Traceless solid-phase synthesis of cyclopenta[c]quinolines and cyclopenta[c]chromenes via hetero [6+3] cycloadditions of fulvene. A facile approach to the 11-heterosteroids framework

AUTHOR(S): Hong, Bor-Cherng; Chen, Zhong-Yi; Chen, Wei-Hung; Sun, Hsu-I.; Lee, Gene-Hsiang

CORPORATE SOURCE: Department of Chemistry and Biochemistry, National Chung Cheng University, Chia-Yi, 621, Taiwan

SOURCE: Journal of the Chinese Chemical Society (Taipei, Taiwan) (2005), 52(1), 181-200
CODEN: JCCTAC; ISSN: 0009-4536

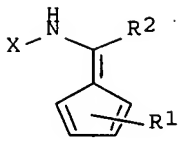
PUBLISHER: Chinese Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:150207

GI



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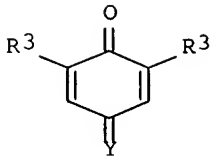
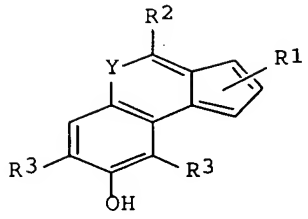


II



III

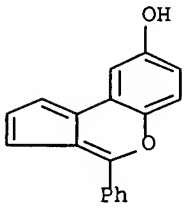
AB The hetero [6+3] cycloaddn. of resin-bound fulvenes I (X = resin; R1 = H, Me; R2 = H, Me, Et, n-Pr, n-Bu, Ph) to benzoquinones and quinonimines, e.g. II (Y = O, 4-Me2NC6H4N; R3 = H, Me, Cl), provides an efficient route to the synthesis of cyclopenta[c]chromenes and cyclopenta[c]quinolines, e.g. III. The structure of the cyclopenta[c]chromene skeleton was confirmed by the X-ray structure anal. of the 4-bromobenzoate of III (Y = O; R1 = H; R2 = R3 = Me). The antiproliferative activity of two cyclopenta[c]chromene derivs. against a number of carcinogenic human cell lines has been studied.

IT **874118-35-1P 874118-44-2P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(solution-phase and traceless solid-phase synthesis of hydroxy-substituted cyclopenta[c]quinolines and cyclopenta[c]chromenes via hetero [6+3] cycloaddns. of fulvenes with quinones or quinonimines)

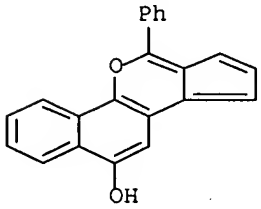
RN 874118-35-1 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 4-phenyl- (9CI) (CA INDEX NAME)



RN 874118-44-2 CAPLUS

CN Cyclopenta[d]naphtho[1,2-b]pyran-11-ol, 6-phenyl- (9CI) (CA INDEX NAME)



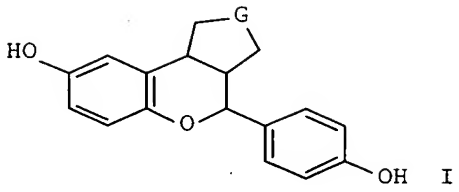
REFERENCE COUNT: 73 THERE ARE 73 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:927190 CAPLUS Full-text
DOCUMENT NUMBER: 141:395410
TITLE: Preparation of substituted benzopyrans as selective estrogen receptor-beta agonists
INVENTOR(S): Durst, Gregory Lee; Norman, Bryan Hurst; Pfeifer, Lance Allen; Richardson, Timothy Ivo
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 129 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2004094400	A2	20041104	WO 2004-US9272		20040408
WO 2004094400	A3	20050224			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 2004232798	A1	20041104	AU 2004-232798		20040408
CA 2518819	A1	20041104	CA 2004-2518819		20040408
EP 1626974	A2	20060222	EP 2004-759767		20040408
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK					
BR 2004009588	A	20060418	BR 2004-9588		20040408
CN 1777614	A	20060524	CN 2004-80010817		20040408
JP 2006524240	T	20061026	JP 2006-509332		20040408
US 2007106082	A1	20070510	US 2005-552504		20051006
MX 2005PA11243	A	20051215	MX 2005-PA11243		20051019
PRIORITY APPLN. INFO.:			US 2003-464404P	P	20030421
			WO 2004-US9272	W	20040408

OTHER SOURCE(S): MARPAT 141:395410
GI



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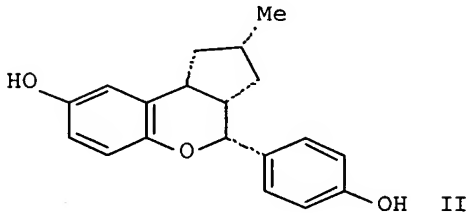


II

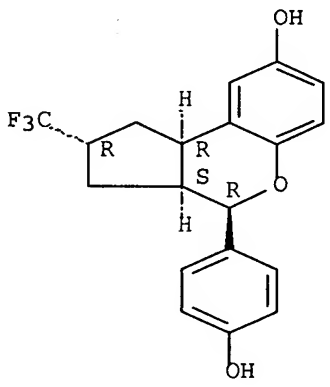
AB Title compds. represented by the formula I [wherein G = CH-alkyl, CO, CHOH, CHCF3, CF2, C(OH)CF3, CH(OH)alkyl, CH-O-alkyl, CHOCO-alkyl, etc; and their enantiomers, and pharmaceutically acceptable salts thereof] were prepared as estrogen receptor (ER)-beta agonists. For example, II was given in a multi-step synthesis starting from hydroquinone. I exhibited binding affinities (Kis) at the ER-α subtype in the range 5.0 - >10,000 nM and to the ER-β subtype in the range of 0.20 - 429 nM. Thus, I and their pharmaceutical compns. are useful as estrogen receptor agonists for the treatment of estrogen receptor mediated diseases such as prostate cancer or benign prostate hyperplasia.

IT **787621-81-2P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

RN 787621-81-2 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-(trifluoromethyl)-, (2R,3aS,4R,9bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

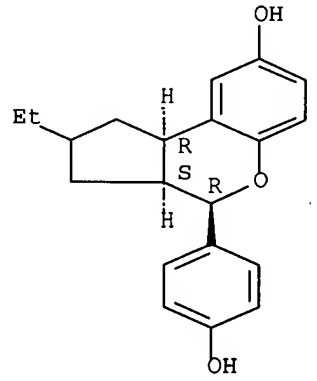


IT **787621-88-9P 787621-99-2P 787622-40-6P**
787622-43-9P 787622-78-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

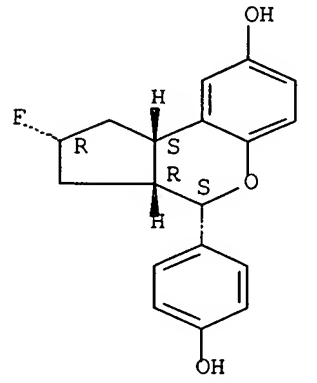
RN 787621-88-9 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 2-ethyl-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



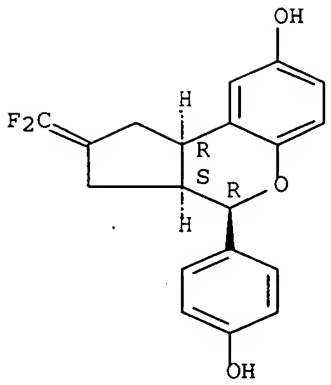
RN 787621-99-2 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 2-fluoro-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (2R,3aR,4S,9bS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



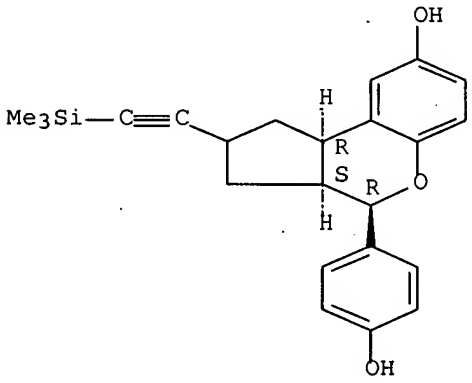
RN 787622-40-6 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 2-(difluoromethylene)-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aS,4R,9bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



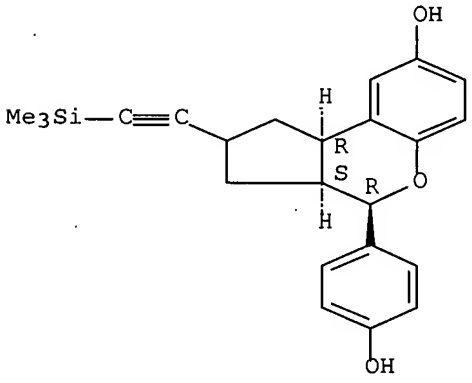
RN 787622-43-9 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-[(trimethylsilyl)ethynyl]-, (3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 787622-78-0 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-[(trimethylsilyl)ethynyl]-, (3aS,4R,9bR)- (9CI) (CA INDEX NAME)

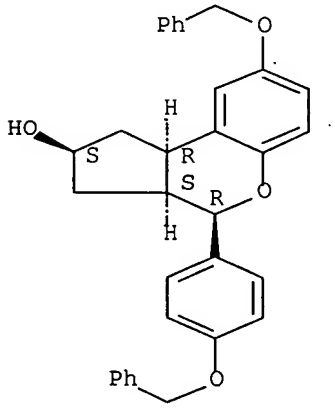
Absolute stereochemistry.



IT 787622-29-1P 787622-41-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

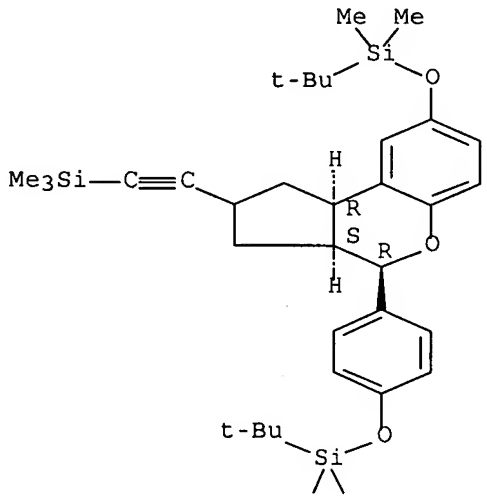
RN 787622-29-1 CAPLUS
CN Cyclopenta[c][1]benzopyran-2-ol, 1,2,3,3a,4,9b-hexahydro-8-(phenylmethoxy)-4-[4-(phenylmethoxy)phenyl]-, (2R,3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 787622-41-7 CAPLUS
CN Silane, (1,1-dimethylethyl)[4-[(3aR,4S,9bS)-8-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1,2,3,3a,4,9b-hexahydro-2-[(trimethylsilyl)ethynyl]cyclopenta[c][1]benzopyran-4-yl]phenoxy]dimethyl-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



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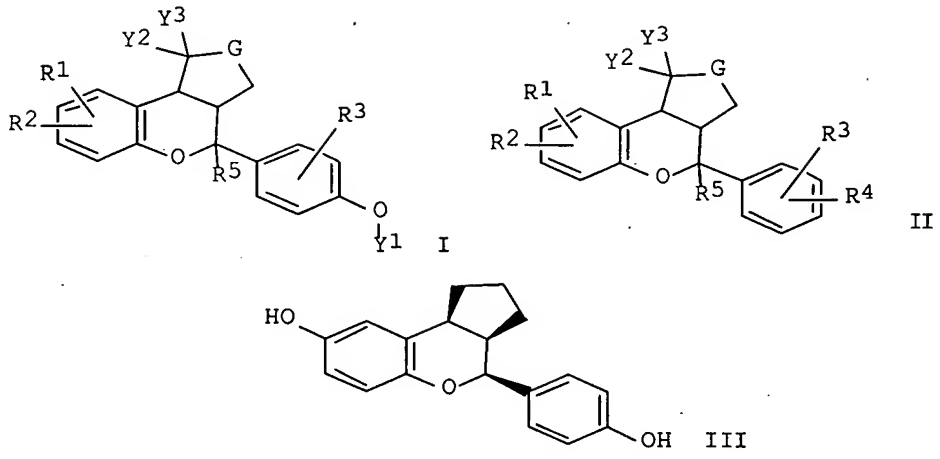
L6 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:417738 CAPLUS Full-text
DOCUMENT NUMBER: 139:6768
TITLE: Preparation of benzopyran derivatives as selective estrogen receptor β agonists
INVENTOR(S): Dodge, Jeffrey Alan; Krishnan, Venkatesh Gary; Lugar, Charles Willis, III; Neubauer, Blake Lee; Norman, Bryan Hurst; Pfeifer, Lance Allen; Richardson, Timothy Ivo
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 138 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003044006	A1	20030530	WO 2002-US33622	20021107
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2467013	A1	20030530	CA 2002-2467013	20021107
AU 2002359283	A1	20030610	AU 2002-359283	20021107
EP 1448544	A1	20040825	EP 2002-793806	20021107
EP 1448544	B1	20070516		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
CN 1589268	A	20050302	CN 2002-822991	20021107
HU 200402628	A2	20050428	HU 2004-2628	20021107
JP 2005513027	T	20050512	JP 2003-545643	20021107
NZ 531850	A	20070126	NZ 2002-531850	20021107
EP 1790644	A1	20070530	EP 2007-102693	20021107
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE, SK, TR, AL, LT, LV, MK, RO, SI				
AT 362471	T	20070615	AT 2002-793806	20021107
US 2004249167	A1	20041209	US 2004-493092	20040420
US 7217734	B2	20070515		
ZA 2004003733	A	20051004	ZA 2004-3733	20040514
IN 2004KN00639	A	20060421	IN 2004-KN639	20040517
MX 2004PA04703	A	20040819	MX 2004-PA4703	20040518
NO 2004002583	A	20040618	NO 2004-2583	20040618
PRIORITY APPLN. INFO.:			US 2001-332766P P	20011119
			US 2002-363622P P	20020311
			EP 2002-793806 A3	20021107

OTHER SOURCE(S): MARPAT 139:6768

GI



AB The title compds. I and II [wherein R1-R4 = independently H, alkyl, OH, alkoxy, halo, amido, or CF3; R5 = H or CF3; Y1-Y3 = independently H or alkyl; G = CH2, CH2CH2, or CH2CH2CH2] and stereoisomers, and pharmaceutical acceptable salts thereof are prepared as selective estrogen receptor β agonists for the treatment of prostate cancer. For example, the benzopyran III was prepared in a multi-step synthesis in moderate yield. III binds to estrogen receptor β (ER β) with a Ki of <1 nM and Ki(ER α)/Ki(ER β) of 8.0.

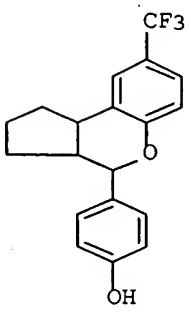
IT **533884-11-6P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of benzopyran derivs. as selective estrogen receptor β agonists)

RN 533884-11-6 CAPLUS

CN Phenol, 4-[1,2,3,3a,4,9b-hexahydro-8-(trifluoromethyl)cyclopenta[c][1]benzopyran-4-yl]- (9CI) (CA INDEX NAME)

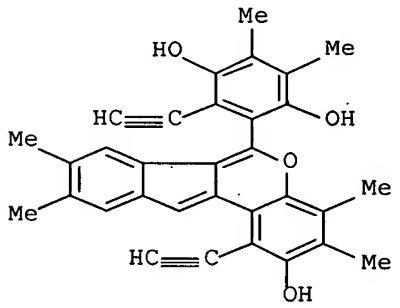


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:689997 CAPLUS Full-text
DOCUMENT NUMBER: 130:38272
TITLE: A novel tandem bicyclization to form an indenopyran ring system
AUTHOR(S): Chakraborty, Manisha; McConville, David B.; Saito, Takeshi; Meng, Huihan; Rinaldi, Peter L.; Tessier, Claire A.; Youngs, Wiley J.
CORPORATE SOURCE: Dep. of Chemistry, University of Akron, Akron, OH, 44325-3601, USA
SOURCE: Tetrahedron Letters (1998), 39(45), 8237-8340
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:38272

AB A new palladium-copper catalyzed intramol. acetylene-zipper type bicyclization between alkyne and hydroxy functionality of an alkynyl hydroquinone has been observed to give a highly conjugated ring system.

IT **216777-12-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of indenopyrans by tandem bicyclization)
RN 216777-12-7 CAPLUS
CN 1,4-Benzenediol, 2-ethynyl-3-(1-ethynyl-2-hydroxy-3,4,8,9-tetramethylbenz[b]indeno[2,1-d]pyran-6-yl)-5,6-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

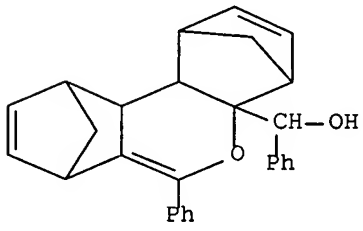
L6 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1972:152831 CAPLUS Full-text
DOCUMENT NUMBER: 76:152831
TITLE: Condensation of phenyl ethynyl ketone with cyclopentadiene. Reinvestigation
AUTHOR(S): Venkataramani, P. S.; Chandrasekharan, S.; Swaminathan, S.
CORPORATE SOURCE: Dep. Org. Chem., Univ. Madras, Madras, India
SOURCE: Tetrahedron (1972), 28(5), 1249-55
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.

AB The earlier structural assignment of 2-benzoylnorborna-diene (I) for the product obtained by the condensation of PhC-(O)C.tplbond.CH with cyclopentadiene is now revised to a dimeric structure, II.

IT **36144-49-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 36144-49-7 CAPLUS

CN 1,4:7,10-Dimethano-4aH-dibenzo[b,d]pyran-4a-methanol, 1,4,7,10,10a,10b-hexahydro-α,6-diphenyl-, [1α,4α,4aβ(R*),7β,10.beta.,10aα,10bβ]- (9CI) (CA INDEX NAME)



L6 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1969:77707 CAPLUS Full-text

DOCUMENT NUMBER: 70:77707

TITLE: Experiments in the brazilane series. I. Preparation of 2-phenyl-5',6',7-trimethoxybrazilane

AUTHOR(S): Morsingh, Francis

CORPORATE SOURCE: Univ. Malaya, Kuala Lumpur, Malay.

SOURCE: Tetrahedron (1969), 25(2), 355-9
CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

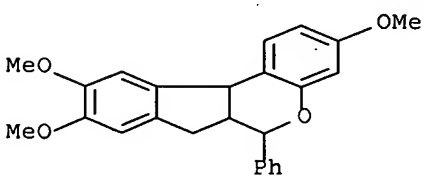
LANGUAGE: English

AB Superposition of flavan on brazilane would afford 2-phenylbrazilane. Although this structure has not yet been isolated, biogenetically it is feasible. The synthesis of 2-phenyl-5',6',7-trimethoxybrazilane is described.

IT **21834-73-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 21834-73-1 CAPLUS

CN Benz[b]indeno[1,2-d]pyran, 6,6a,7,11b-tetrahydro-3,9,10-trimethoxy-6-phenyl- (8CI) (CA INDEX NAME)



L6 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1946:23981 CAPLUS Full-text

DOCUMENT NUMBER: 40:23981

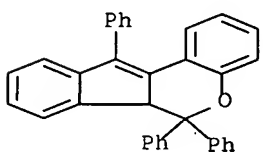
ORIGINAL REFERENCE NO.: 40:4709e-i,4710a-b
TITLE: Condensation of tetraphenylbutynediol with phenol
AUTHOR(S): Zal'kind, Yu. S.; Teterin, V. K.; Kuznetsov, S. G.
CORPORATE SOURCE: Leningrad Chem. Tech. Inst.
SOURCE: Zhurnal Obshchei Khimii (1945), 15, 488-98
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB [.tplbond.CC(OH)Ph2]2 (I) (30 g.), 87.6 g. PhOH, 60 cc. benzene and 0.4 g. dry H2NC6H4SO3H were refluxed for 2 h. with continuous removal of water by means of a Stark-Dean type collector, in which 3.35 cc. H2O was collected at the end of the reaction; after cooling and dilution with benzene, the crystalline and the liquid portions were steam-distilled to remove the solvent. There were obtained 28.7 g. crystalline matter and 16.7 g. red resin. Prolonged recrystn. from benzene, CHCl3, and ligroin gave the following products: 21.5 g. 1-diphenylmethylene-2-p-hydroxyphenyl-3-phenylindene, m. 255° (II), yellow-orange needles; 2.8 g. 1-diphenylmethylene-2- phenoxy-3-phenylindene (III), m. 223°, orange prisms; 1.2 g. 2,2,5,5-tetraphenyl-3-phenoxy-2,5-dihydrofuran, m. 176°, colorless needles; and 0.4 g. 2,2,3'-triphenyl-1',2',3,4-indenochroman (IV), m. 216-17°, colorless parallelopipeds. II was converted into the MeO derivative, m. 176-7 °, by boiling with MeI in the presence of K2CO3 in Me2CO, or by treatment with Me2SO4 in 20% NaOH; rapid crystallization from Me2CO leads to yellow needles of the above m.p., slow crystallization gives large red-brown parallelopipeds, m. 167-8°. III was prepared by an alternate method for identification: 10.5 g. I in 150 cc. Et2O was treated with 22.5 g. PCl3 at 1°over 5 h., stirred for 2 h. at 0° and for 4 h. at room temperature to yield, after removal of the solvent, hydrolysis, and crystallization from ligroin 1.0 g. 1-diphenylmethylene-2-chloro-3- phenylindene, m. 157° (cf. Wieland and Kloss, C.A. 23, 3696), and 3 unidentified products m. 147-8° (4.5 g.), m. 194-5° (0.2 g.), and m. 165° (0.4 g.); 0.4 g. of the chloride was added to a solution of 0.1 g. K in 2 g. molten PhOH and heated slowly to 220° for 1 h.; after treatment with alkaline water, extraction of the precipitate with EtOH, and crystallization of the residue from benzene-petr. ether there was obtained a product identical with III, m. 223°, above. Boiling of this in MePh in the presence of sulfanilic acid failed to effect any isomerization. IV on boiling with alc. KOH is transformed into 2 substances which were unidentified: colorless, m. 230° (from EtOH, then EtOHMe2CO), and orange, m. 208-19°, with the former transforming into a product m. 208-14°, on heating above the m.p. The condensation of I with PhOH was also conducted in the presence of the following catalysts: activated Chasoviarskii clay, H2SO4-AcOH, and glacial AcOH. The 1st catalyst gave results similar to sulfanilic acid while the 2nd catalyst gave only II, m. 255°, in 98% yield (crude); the 3rd catalyst gave only a resinous, ill-defined mixture of some transformation products of the glycol without condensation with PhOH.

IT **860186-11-4P**, Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11-triphenyl-
RL: PREP (Preparation)
(preparation of)

RN 860186-11-4 CAPLUS

CN Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11-triphenyl- (4CI) (CA INDEX NAME)



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FULL ESTIMATED COST                                   101.43     115.59

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                   -10.92     -10.92

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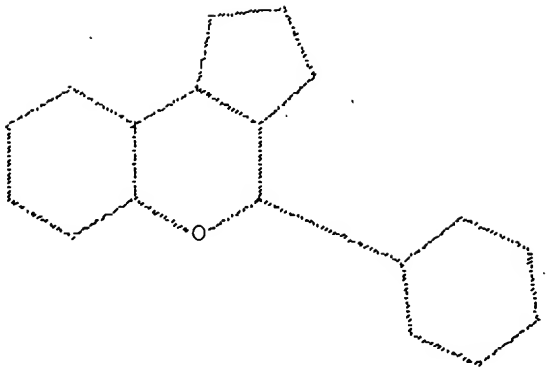

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED -     1636 TO ITERATE

100.0% PROCESSED     1636 ITERATIONS                                 17 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        30294 TO    35146
PROJECTED ANSWERS:              93 TO      587

L8            17 SEA SSS SAM L7

=> d scan

L8   17 ANSWERS   REGISTRY  COPYRIGHT 2007 ACS on STN
IN   Cyclopenta[c][1]benzopyran-8-ol, 4-phenyl- (9CI)
MF   C18 H12 O2
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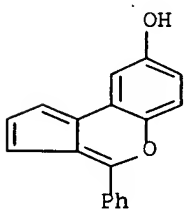


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HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L8   17 ANSWERS   REGISTRY  COPYRIGHT 2007 ACS on STN
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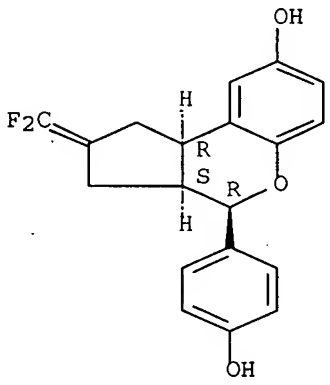
IN Cyclopenta[c][1]benzopyran-8-ol, 2-(difluoromethylene)-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aS,4R,9bR)- (9CI)
MF C19 H16 F2 O3

Absolute stereochemistry.



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100.0% PROCESSED 31330 ITERATIONS 281 ANSWERS
SEARCH TIME: 00.00.01

L9 281 SEA SSS FUL L7

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COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID
The query entered contains both search terms created by structure-building or screen commands and text search terms. L#s created via the STRUCTURE or SCREEN commands must be searched in the structures files separately from text terms or profiles. The L# answer sets from structure searches can be used in crossover searches and can be combined with text terms.

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=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION

FULL ESTIMATED COST 175.25 290.84

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY TOTAL SESSION

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Substance data SEARCH and crossover from CAS REGISTRY in progress...
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SAMPLE SCREEN SEARCH COMPLETED - 1636 TO ITERATE

100.0% PROCESSED 1636 ITERATIONS 17 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 30294 TO 35146
PROJECTED ANSWERS: 93 TO 587

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L12 8 L11

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4212934 PRY<2004

L13 6 L12 AND (PY<2004 OR AY<2004 OR PRY<2004)

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L13 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:927190 CAPLUS Full-text
DOCUMENT NUMBER: 141:395410
TITLE: Preparation of substituted benzopyrans as selective estrogen receptor-beta agonists
INVENTOR(S): Durst, Gregory Lee; Norman, Bryan Hurst; Pfeifer, Lance Allen; Richardson, Timothy Ivo
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 129 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
WO 2004094400	A2	20041104	WO 2004-US9272		20040408	<--
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AU 2004232798	A1	20041104	AU 2004-232798		20040408	<--
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OTHER SOURCE(S): MARPAT 141:395410
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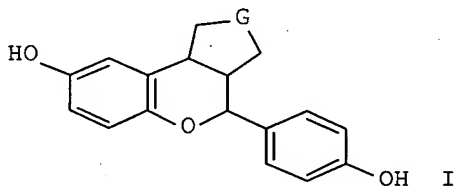

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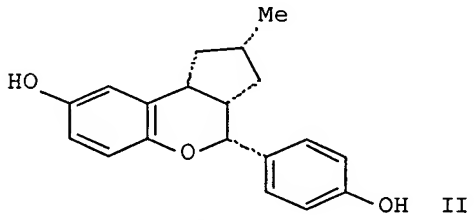


II

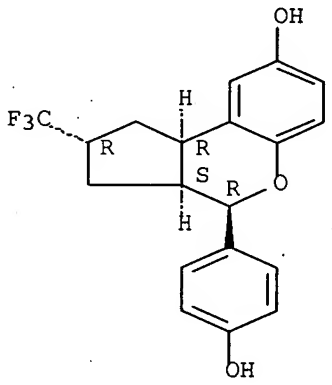
AB Title compds. represented by the formula I [wherein G = CH-alkyl, CO, CHOH, CHCF3, CF2, C(OH)CF3, CH(OH)alkyl, CH-O-alkyl, CHOCO-alkyl, etc; and their enantiomers, and pharmaceutically acceptable salts thereof] were prepared as estrogen receptor (ER)-beta agonists. For example, II was given in a multi-step synthesis starting from hydroquinone. I exhibited binding affinities (Kis) at the ER-α subtype in the range 5.0 - >10,000 nM and to the ER-β subtype in the range of 0.20 - 429 nM. Thus, I and their pharmaceutical compns. are useful as estrogen receptor agonists for the treatment of estrogen receptor mediated diseases such as prostate cancer or benign prostate hyperplasia.

IT **787621-81-2P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

RN 787621-81-2 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-(trifluoromethyl)-, (2R,3aS,4R,9bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

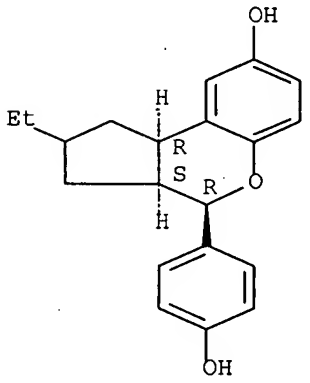


IT **787621-88-9P 787621-99-2P 787622-40-6P**
787622-43-9P 787622-78-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

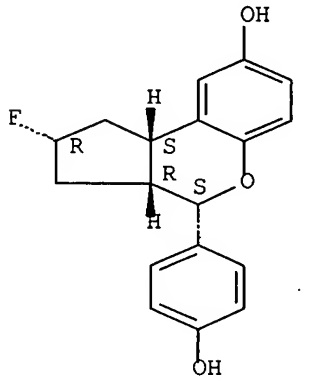
RN 787621-88-9 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 2-ethyl-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



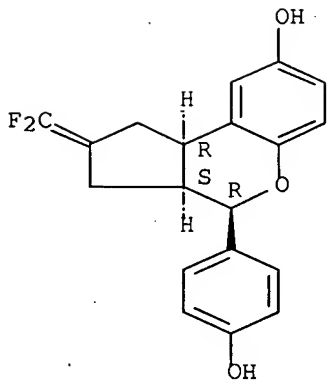
RN 787621-99-2 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 2-fluoro-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (2R,3aR,4S,9bS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



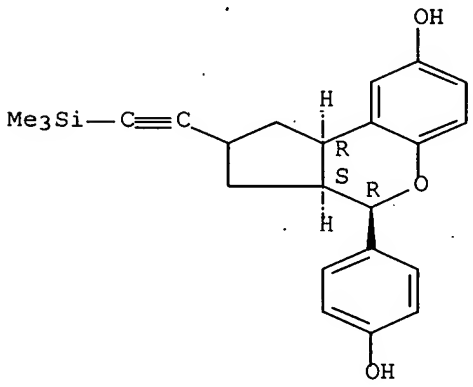
RN 787622-40-6 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 2-(difluoromethylene)-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aS,4R,9bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



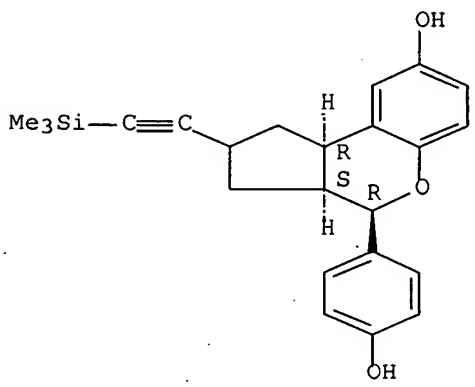
RN 787622-43-9 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-[(trimethylsilyl)ethynyl]-, (3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 787622-78-0 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-[(trimethylsilyl)ethynyl]-, (3aS,4R,9bR)- (9CI) (CA INDEX NAME)

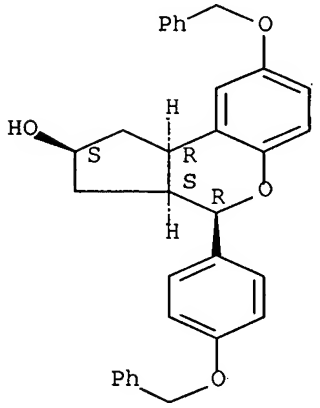
Absolute stereochemistry.



IT 787622-29-1P 787622-41-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

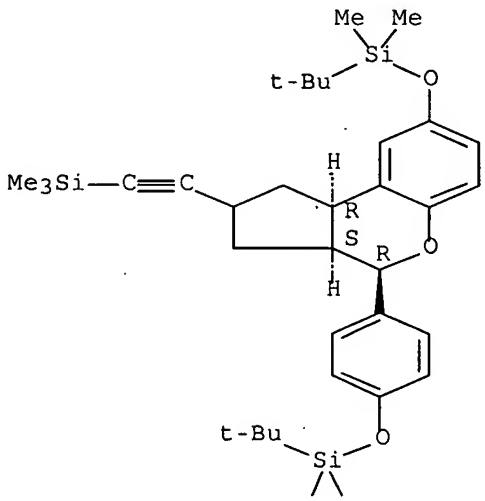
RN 787622-29-1 CAPLUS
CN Cyclopenta[c][1]benzopyran-2-ol, 1,2,3,3a,4,9b-hexahydro-8-(phenylmethoxy)-4-[4-(phenylmethoxy)phenyl]-, (2R,3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 787622-41-7 CAPLUS
CN Silane, (1,1-dimethylethyl)[4-[(3aR,4S,9bS)-8-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1,2,3,3a,4,9b-hexahydro-2-[(trimethylsilyl)ethynyl]cyclopenta[c][1]benzopyran-4-yl]phenoxy]dimethyl-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



Me Me

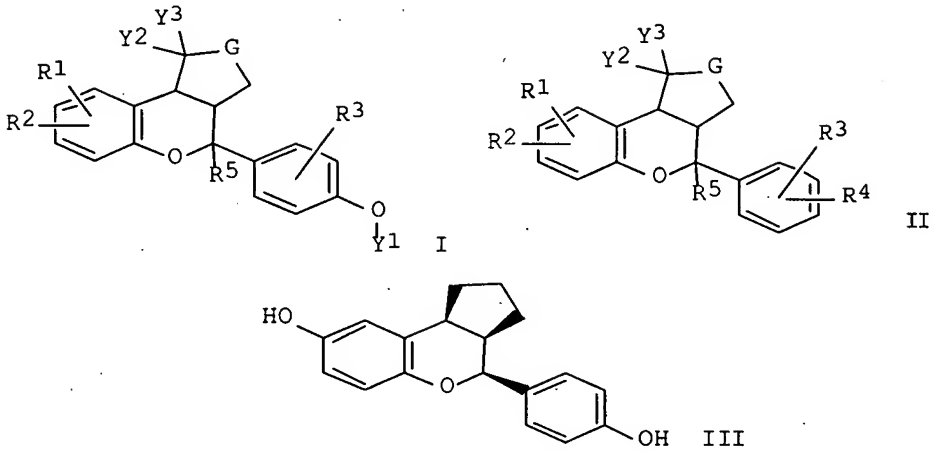
L13 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:417738 CAPLUS Full-text
DOCUMENT NUMBER: 139:6768
TITLE: Preparation of benzopyran derivatives as selective estrogen receptor β agonists
INVENTOR(S): Dodge, Jeffrey Alan; Krishnan, Venkatesh Gary; Lugar, Charles Willis, III; Neubauer, Blake Lee; Norman, Bryan Hurst; Pfeifer, Lance Allen; Richardson, Timothy Ivo
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 138 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003044006	A1	20030530	WO 2002-US33622	20021107 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2467013	A1	20030530	CA 2002-2467013	20021107 <--
AU 2002359283	A1	20030610	AU 2002-359283	20021107 <--
EP 1448544	A1	20040825	EP 2002-793806	20021107 <--
EP 1448544	B1	20070516		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
CN 1589268	A	20050302	CN 2002-822991	20021107 <--
HU 200402628	A2	20050428	HU 2004-2628	20021107 <--
JP 2005513027	T	20050512	JP 2003-545643	20021107 <--
NZ 531850	A	20070126	NZ 2002-531850	20021107 <--
EP 1790644	A1	20070530	EP 2007-102693	20021107 <--
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE, SK, TR, AL, LT, LV, MK, RO, SI				
AT 362471	T	20070615	AT 2002-793806	20021107 <--
US 2004249167	A1	20041209	US 2004-493092	20040420 <--
US 7217734	B2	20070515		
ZA 2004003733	A	20051004	ZA 2004-3733	20040514 <--
IN 2004KN00639	A	20060421	IN 2004-KN639	20040517 <--
MX 2004PA04703	A	20040819	MX 2004-PA4703	20040518 <--
NO 2004002583	A	20040618	NO 2004-2583	20040618 <--
PRIORITY APPLN. INFO.:			US 2001-332766P P	20011119 <--
			US 2002-363622P P	20020311 <--
			EP 2002-793806 A3	20021107 <--

WO 2002-US33622 W 20021107 <--

OTHER SOURCE(S): MARPAT 139:6768

GI



I II

III

AB The title compds. I and II [wherein R1-R4 = independently H, alkyl, OH, alkoxy, halo, amido, or CF3; R5 = H or CF3; Y1-Y3 = independently H or alkyl; G = CH2, CH2CH2, or CH2CH2CH2] and stereoisomers, and pharmaceutical acceptable salts thereof are prepared as selective estrogen receptor β agonists for the treatment of prostate cancer. For example, the benzopyran III was prepared in a multi-step synthesis in moderate yield. III binds to estrogen receptor β (ER β) with a Ki of <1 nM and Ki(ER α)/Ki(ER β) of 8.0.

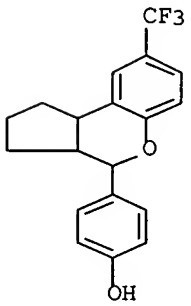
IT **533884-11-6P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of benzopyran derivs. as selective estrogen receptor β agonists)

RN 533884-11-6 CAPLUS

CN Phenol, 4-[1,2,3,3a,4,9b-hexahydro-8-(trifluoromethyl)cyclopenta[c][1]benzopyran-4-yl]- (9CI) (CA INDEX NAME)

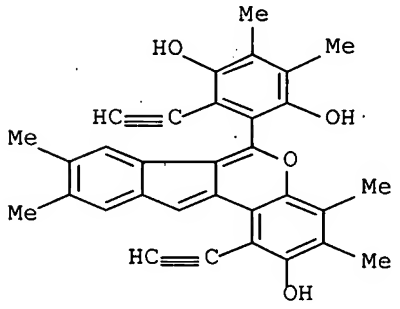


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:689997 CAPLUS Full-text
DOCUMENT NUMBER: 130:38272
TITLE: A novel tandem bicyclization to form an indenopyran ring system
AUTHOR(S): Chakraborty, Manisha; McConville, David B.; Saito, Takeshi; Meng, Huihan; Rinaldi, Peter L.; Tessier, Claire A.; Youngs, Wiley J.
CORPORATE SOURCE: Dep. of Chemistry, University of Akron, Akron, OH, 44325-3601, USA
SOURCE: Tetrahedron Letters (1998), 39(45), 8237-8340
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:38272

AB A new palladium-copper catalyzed intramol. acetylene-zipper type bicyclization between alkyne and hydroxy functionality of an alkynyl hydroquinone has been observed to give a highly conjugated ring system.

IT **216777-12-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of indenopyrans by tandem bicyclization)
RN 216777-12-7 CAPLUS
CN 1,4-Benzenediol, 2-ethynyl-3-(1-ethynyl-2-hydroxy-3,4,8,9-tetramethylbenz[b]indeno[2,1-d]pyran-6-yl)-5,6-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

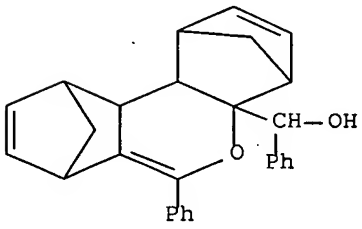
L13 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1972:152831 CAPLUS Full-text
DOCUMENT NUMBER: 76:152831
TITLE: Condensation of phenyl ethynyl ketone with cyclopentadiene. Reinvestigation
AUTHOR(S): Venkataramani, P. S.; Chandrasekharan, S.; Swaminathan, S.
CORPORATE SOURCE: Dep. Org. Chem., Univ. Madras, Madras, India
SOURCE: Tetrahedron (1972), 28(5), 1249-55
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.

AB The earlier structural assignment of 2-benzoylnorborna-diene (I) for the product obtained by the condensation of PhC-(O)C.tplbond.CH with cyclopentadiene is now revised to a dimeric structure, II.

IT **36144-49-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 36144-49-7 CAPLUS

CN 1,4:7,10-Dimethano-4aH-dibenzo[b,d]pyran-4a-methanol, 1,4,7,10,10a,10b-hexahydro-α,6-diphenyl-, [1α,4α,4aβ(R*),7β,10.beta.,10aα,10bβ]- (9CI) (CA INDEX NAME)



L13 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1969:77707 CAPLUS Full-text

DOCUMENT NUMBER: 70:77707

TITLE: Experiments in the brazilane series. I. Preparation of 2-phenyl-5',6',7-trimethoxybrazilane

AUTHOR(S): Morsingh, Francis

CORPORATE SOURCE: Univ. Malaya, Kuala Lumpur, Malay.

SOURCE: Tetrahedron (1969), 25(2), 355-9
CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

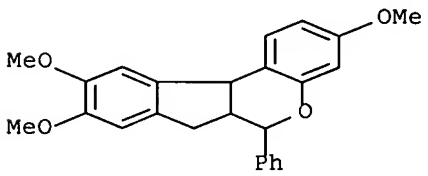
LANGUAGE: English

AB Superposition of flavan on brazilane would afford 2-phenylbrazilane. Although this structure has not yet been isolated, biogenetically it is feasible. The synthesis of 2-phenyl-5',6',7-trimethoxybrazilane is described.

IT **21834-73-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 21834-73-1 CAPLUS

CN Benz[b]indeno[1,2-d]pyran, 6,6a,7,11b-tetrahydro-3,9,10-trimethoxy-6-phenyl- (8CI) (CA INDEX NAME)



L13 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1946:23981 CAPLUS Full-text

DOCUMENT NUMBER: 40:23981

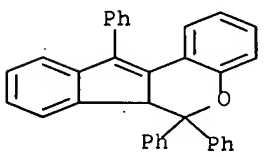
ORIGINAL REFERENCE NO.: 40:4709e-i,4710a-b
TITLE: Condensation of tetraphenylbutynediol with phenol
AUTHOR(S): Zal'kind, Yu. S.; Teterin, V. K.; Kuznetsov, S. G.
CORPORATE SOURCE: Leningrad Chem. Tech. Inst.
SOURCE: Zhurnal Obshchei Khimii (1945), 15, 488-98
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB [.tplbond.CC(OH)Ph2]2 (I) (30 g.), 87.6 g. PhOH, 60 cc. benzene and 0.4 g. dry H2NC6H4SO3H were refluxed for 2 h. with continuous removal of water by means of a Stark-Dean type collector, in which 3.35 cc. H2O was collected at the end of the reaction; after cooling and dilution with benzene, the crystalline and the liquid portions were steam-distilled to remove the solvent. There were obtained 28.7 g. crystalline matter and 16.7 g. red resin. Prolonged recrystn. from benzene, CHCl3, and ligroin gave the following products: 21.5 g. 1-diphenylmethylene-2-p-hydroxyphenyl-3-phenylindene, m. 255° (II), yellow-orange needles; 2.8 g. 1-diphenylmethylene-2- phenoxy-3-phenylindene (III), m. 223°, orange prisms; 1.2 g. 2,2,5,5-tetraphenyl-3-phenoxy-2,5-dihydrofuran, m. 176°, colorless needles; and 0.4 g. 2,2,3'-triphenyl-1',2',3,4-indenochroman (IV), m. 216-17°, colorless parallelopipeds. II was converted into the MeO derivative, m. 176-7 °, by boiling with MeI in the presence of K2CO3 in Me2CO, or by treatment with Me2SO4 in 20% NaOH; rapid crystallization from Me2CO leads to yellow needles of the above m.p., slow crystallization gives large red-brown parallelopipeds, m. 167-8°. III was prepared by an alternate method for identification: 10.5 g. I in 150 cc. Et2O was treated with 22.5 g. PCl3 at 1°over 5 h., stirred for 2 h. at 0° and for 4 h. at room temperature to yield, after removal of the solvent, hydrolysis, and crystallization from ligroin 1.0 g. 1-diphenylmethylene-2-chloro-3- phenylindene, m. 157° (cf. Wieland and Kloss, C.A. 23, 3696), and 3 unidentified products m. 147-8° (4.5 g.), m. 194-5° (0.2 g.), and m. 165° (0.4 g.); 0.4 g. of the chloride was added to a solution of 0.1 g. K in 2 g. molten PhOH and heated slowly to 220° for 1 h.; after treatment with alkaline water, extraction of the precipitate with EtOH, and crystallization of the residue from benzene-petr. ether there was obtained a product identical with III, m. 223°, above. Boiling of this in MePh in the presence of sulfanilic acid failed to effect any isomerization. IV on boiling with alc. KOH is transformed into 2 substances which were unidentified: colorless, m. 230° (from EtOH, then EtOHMe2CO), and orange, m. 208-19°, with the former transforming into a product m. 208-14°, on heating above the m.p. The condensation of I with PhOH was also conducted in the presence of the following catalysts: activated Chasoviarskii clay, H2SO4-AcOH, and glacial AcOH. The 1st catalyst gave results similar to sulfanilic acid while the 2nd catalyst gave only II, m. 255°, in 98% yield (crude); the 3rd catalyst gave only a resinous, ill-defined mixture of some transformation products of the glycol without condensation with PhOH.

IT **860186-11-4P**, Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11-triphenyl-
RL: PREP (Preparation)
(preparation of)

RN 860186-11-4 CAPLUS

CN Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11-triphenyl- (4CI) (CA INDEX NAME)



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=>

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* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

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 NEWS  4  MAY 14   RDISCLOSURE on STN Easy enhanced with new search and display
                   fields
 NEWS  5  MAY 21   BIOSIS reloaded and enhanced with archival data
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 NEWS  7  MAY 21   CA/CAplus enhanced with additional kind codes for German
                   patents
 NEWS  8  MAY 22   CA/CAplus enhanced with IPC reclassification in Japanese
                   patents
 NEWS  9  JUN 27   CA/CAplus enhanced with pre-1967 CAS Registry Numbers
 NEWS 10  JUN 29   STN Viewer now available
 NEWS 11  JUN 29   STN Express, Version 8.2, now available
 NEWS 12  JUL 02   LEMBASE coverage updated
 NEWS 13  JUL 02   LMEDLINE coverage updated
 NEWS 14  JUL 02   SCISEARCH enhanced with complete author names
 NEWS 15  JUL 02   CHEMCATS accession numbers revised
 NEWS 16  JUL 02   CA/CAplus enhanced with utility model patents from China
 NEWS 17  JUL 16   CAplus enhanced with French and German abstracts
 NEWS 18  JUL 18   CA/CAplus patent coverage enhanced
 NEWS 19  JUL 26   USPATFULL/USPAT2 enhanced with IPC reclassification
 NEWS 20  JUL 30   USGENE now available on STN
 NEWS 21  AUG 06   CAS REGISTRY enhanced with new experimental property tags
 NEWS 22  AUG 06   BEILSTEIN updated with new compounds
 NEWS 23  AUG 06   FSTA enhanced with new thesaurus edition

 NEWS EXPRESS  29 JUNE 2007:  CURRENT WINDOWS VERSION IS V8.2,
               CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.

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FILE 'HOME' ENTERED AT 14:26:13 ON 06 AUG 2007

=> file reg
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 0.21 0.21

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DICTIONARY FILE UPDATES: 5 AUG 2007 HIGHEST RN 944042-79-9

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L1 STRUCTURE UPLOADED

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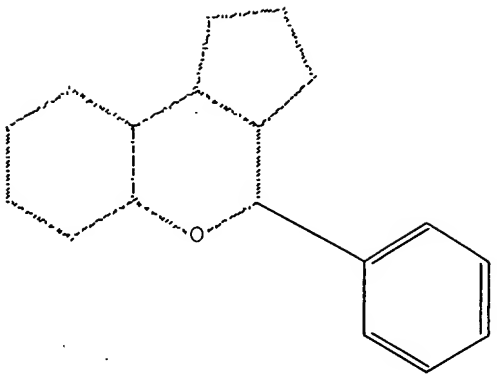
L1 STR



Structure attributes must be viewed using STN Express query preparation.

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100.0% PROCESSED     1636 ITERATIONS                                 17 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        30294 TO    35146
PROJECTED ANSWERS:              93 TO      587

L2            17 SEA SSS SAM L1

=> d scan

L2    17 ANSWERS   REGISTRY  COPYRIGHT 2007 ACS on STN
IN    Cyclopenta[c][1]benzopyran-8-ol, 2-fluoro-1,2,3,3a,4,9b-hexahydro-4-(4-
      hydroxyphenyl)-, (2R,3aR,4S,9bS)- (9CI)
MF    C18 H17 F O3

Absolute stereochemistry.
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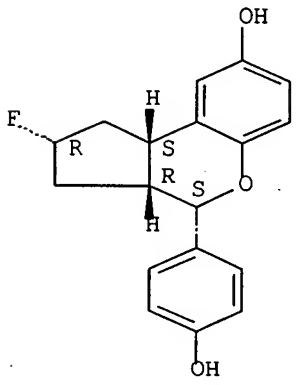
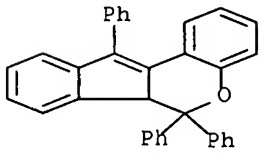


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

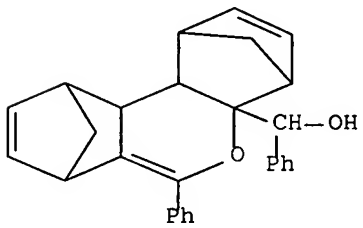
L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11-triphenyl- (4CI)
MF C34 H24 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 1,4:7,10-Dimethano-4aH-dibenzo[b,d]pyran-4a-methanol, 1,4,7,10,10a,10b-hexahydro-α,6-diphenyl-, [1α,4α,4aβ(R*),7β,10.beta.,10aα,10bβ]- (9CI)
MF C28 H26 O2

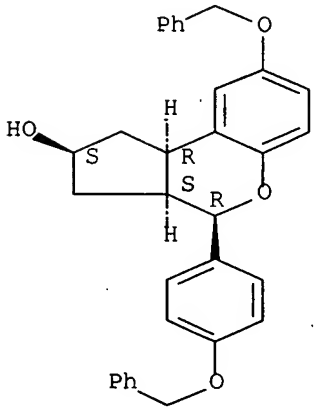


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Cyclopenta[c][1]benzopyran-2-ol, 1,2,3,3a,4,9b-hexahydro-8-(phenylmethoxy)-4-[4-(phenylmethoxy)phenyl]-, (2R,3aR,4S,9bS)-rel- (9CI)
MF C32 H30 O4

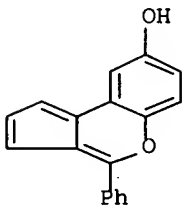
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

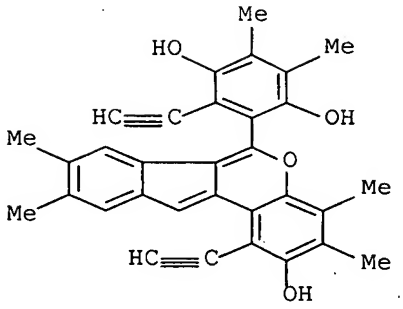
L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Cyclopenta[c][1]benzopyran-8-ol, 4-phenyl- (9CI)
MF C18 H12 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 1,4-Benzenediol, 2-ethynyl-3-(1-ethynyl-2-hydroxy-3,4,8,9-tetramethylbenz[b]indeno[2,1-d]pyran-6-yl)-5,6-dimethyl- (9CI)
MF C32 H26 O4

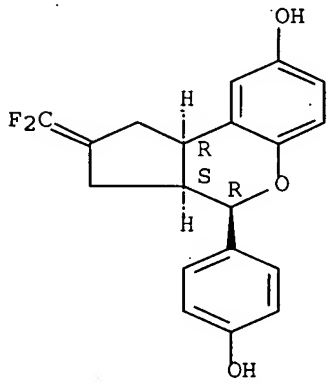


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Cyclopenta[c][1]benzopyran-8-ol, 2-(difluoromethylene)-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aS,4R,9bR)- (9CI)
MF C19 H16 F2 O3

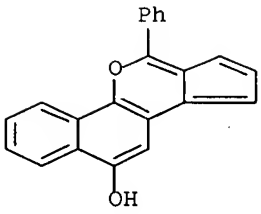
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

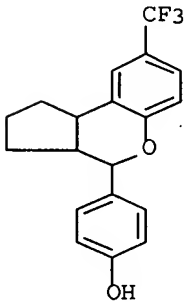
L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Cyclopenta[d]naphtho[1,2-b]pyran-11-ol, 6-phenyl- (9CI)
MF C22 H14 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Phenol, 4-[1,2,3,3a,4,9b-hexahydro-8-(trifluoromethyl)cyclopenta[c][1]benzopyran-4-yl]- (9CI)
MF C19 H17 F3 O2



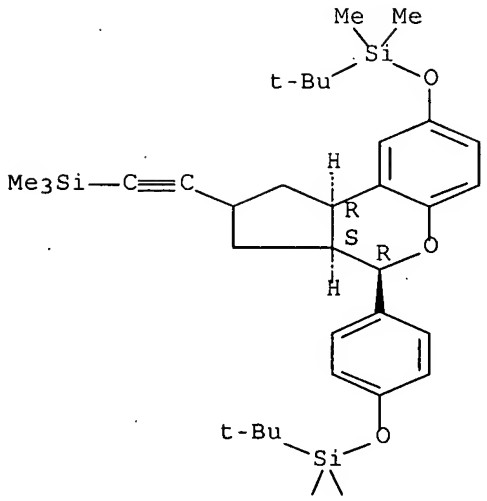
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Silane, (1,1-dimethylethyl)[4-[(3aR,4S,9bS)-8-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1,2,3,3a,4,9b-hexahydro-2-[(trimethylsilyl)ethynyl]cyclopenta[c][1]benzopyran-4-yl]phenoxy]dimethyl-, rel- (9CI)
MF C35 H54 O3 Si3

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

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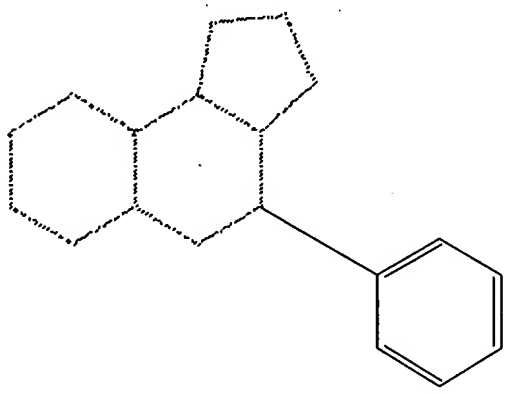
L3 STRUCTURE UPLOADED

=> d l3
L3 HAS NO ANSWERS
L3 STR



Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED -     2835 TO ITERATE

 70.5% PROCESSED     2000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        53507 TO    59893
PROJECTED ANSWERS:               0 TO        0

L4             0 SEA SSS SAM L3

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                                13.95      14.16

FILE 'CAPLUS' ENTERED AT 14:45:00 ON 06 AUG 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 6 Aug 2007  VOL 147 ISS 7
FILE LAST UPDATED: 5 Aug 2007  (20070805/ED)

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They are available for your review at:

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=> s l2 and (py<2004 or ay<2004 or pry<2004)
             8 L2
      23927525 PY<2004
       4731037 AY<2004
       4212934 PRY<2004
L5             6 L2 AND (PY<2004 OR AY<2004 OR PRY<2004)

=> d scan

L5    6 ANSWERS   CAPLUS  COPYRIGHT 2007 ACS on STN
IC   ICM  C07D311-00
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CC 27-7 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 63

TI Preparation of substituted benzopyrans as selective estrogen receptor-beta agonists

ST benzopyran prepn estrogen receptor beta agonist anticancer

IT Prostate gland, disease
(benign hyperplasia; preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

IT Hyperplasia
(benign prostatic; preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

IT Human
Prostate gland, neoplasm
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

IT Antitumor agents
(prostate gland; preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

IT Estrogen receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(β; preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

IT **787621-59-4P** **787621-60-7P** **787621-80-1P** **787621-81-2P**
787622-06-4P **787622-10-0P** **787622-73-5P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

IT **787621-53-8P** **787621-54-9P** **787621-55-0P** **787621-56-1P** **787621-57-2P**
787621-58-3P **787621-61-8P** **787621-62-9P** **787621-63-0P** **787621-64-1P**
787621-69-6P **787621-72-1P** **787621-73-2P** **787621-75-4P** **787621-77-6P**
787621-78-7P **787621-82-3P** **787621-83-4P** **787621-85-6P** **787621-86-7P**
787621-88-9P **787621-90-3P** **787621-91-4P** **787621-93-6P**
787621-94-7P **787621-96-9P** **787621-97-0P** **787621-98-1P**
787621-99-2P **787622-11-1P** **787622-13-3P** **787622-22-4P**
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

IT 62-23-7, p-Nitrobenzoic acid 75-86-5, Acetone cyanohydrin 96-33-3, Methyl acrylate 96-35-5, Methyl glycolate 100-39-0, Benzyl bromide 123-31-9, Hydroquinone, reactions 623-82-5, (R)-(+)-3-Methyladipic acid 892-20-6, Triphenyltin hydride 1066-54-2, Trimethylsilylacetylene 1100-88-5, Benzyltriphenylphosphonium chloride 1530-32-1, Ethyltriphenylphosphonium bromide 2365-48-2, Methyl thioglycolate 2622-05-1, Allylmagnesium chloride 3058-01-3, 3-Methyladipic acid 5781-53-3, Methyl chloroglyoxylate 6228-47-3, Propyltriphenylphosphonium bromide 6793-92-6, p-Benzyloxybromobenzene 10347-88-3, 3-tert-Butyladipic acid 10538-51-9, 2,5-Dimethoxycinnamic acid

22444-89-9, Butyltriphenylphosphonium 25458-45-1, 1-Bromo-4-(methoxymethoxy)benzene 37595-74-7, N-Phenyltrifluoromethanesulfonimide 38053-91-7, 2-[(Trimethylsilyl)oxy]butadiene 38078-09-0, N,N-Diethylaminosulfur trifluoride 70160-51-9 72047-94-0, [2-(Acetoxymethyl)allyl]trimethylsilane 108270-19-5 146631-00-7, 4-(Benzyloxy)phenylboronic acid 787622-05-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

IT 2689-68-1P 4463-74-5P 6093-68-1P, 6-Hydroxycoumarin 57595-23-0P 87905-74-6P, 1,4-Bis(methoxymethoxy)benzene 608536-53-4P, 6-Methoxymethoxycoumarin 787621-46-9P 787621-47-0P 787621-48-1P 787621-49-2P 787621-50-5P 787621-51-6P 787621-52-7P 787621-65-2P 787621-66-3P 787621-67-4P 787621-68-5P 787621-70-9P 787621-71-0P 787621-74-3P 787621-76-5P 787621-79-8P 787621-84-5P 787621-87-8P 787621-89-0P 787621-92-5P 787621-95-8P 787622-00-8P 787622-01-9P 787622-02-0P 787622-03-1P 787622-04-2P 787622-07-5P 787622-08-6P 787622-09-7P 787622-12-2P 787622-14-4P 787622-15-5P 787622-16-6P 787622-18-8P 787622-19-9P 787622-20-2P 787622-21-3P 787622-23-5P, 6-Benzyloxychromen-2-one 787622-25-7P 787622-26-8P 787622-27-9P 787622-28-0P **787622-29-1P** 787622-30-4P 787622-35-9P 787622-38-2P **787622-41-7P** 787622-45-1P 787622-46-2P 787622-47-3P 787622-48-4P 787622-60-0P 787622-61-1P 787622-62-2P 787622-63-3P 787622-64-4P 787622-65-5P 787622-66-6P 787622-67-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L5 6 ANSWERS CAPLUS COPYRIGHT 2007 ACS on STN
CC 10 (Organic Chemistry)
TI Condensation of tetraphenylbutynediol with phenol
IT Catalysts
(for condensation, of PhOH with 1,1,4,4-tetraphenyl-2-butyne-1,4-diol)
IT 411220-98-9P, Indene, 1-benzohydrylidene-2-chloro-3-phenyl- 411220-98-9P, Methane, (2-chloro-3-phenyl-1-indenylidene)diphenyl- 854748-48-4P, Methane, [2-(p-methoxyphenyl)-3-phenyl-1-indenylidene]diphenyl- 854748-48-4P, Anisole, p-(1-benzohydrylidene-3-phenyl-2-indenyl)- 854748-48-4P, Indene, 1-benzohydrylidene-2-(p-methoxyphenyl)-3-phenyl- 854749-76-1P, Indene, 1-benzohydrylidene-2-phenoxy-3-phenyl- 854749-76-1P, Methane, (2-phenoxy-3-phenyl-1-indenylidene)diphenyl- 860000-10-8P, Furan, 2,5-dihydro-3-phenoxy-2,2,5,5-tetraphenyl- **860186-11-4P**, Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11-triphenyl- 861008-63-1P, Phenol, p-(1-benzohydrylidene-3-phenyl-2-indenyl)-
RL: PREP (Preparation)
(preparation of)
IT 1483-74-5, 2-Butyne-1,4-diol, tetraphenyl-
(reaction with phenol)
IT 108-95-2, Phenol
(reactions of, with 1,1,4,4-tetraphenyl-2-butyne-1,4-diol)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> d ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 6 ANSWERS - CONTINUE? Y/(N):y

L5 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:927190 CAPLUS Full-text
DOCUMENT NUMBER: 141:395410
TITLE: Preparation of substituted benzopyrans as selective estrogen receptor-beta agonists
INVENTOR(S): Durst, Gregory Lee; Norman, Bryan Hurst; Pfeifer, Lance Allen; Richardson, Timothy Ivo
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 129 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
WO 2004094400	A2	20041104	WO 2004-US9272		20040408	<--
WO 2004094400	A3	20050224				
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW						
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG						
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US 2007106082	A1	20070510	US 2005-552504		20051006	<--
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PRIORITY APPLN. INFO.:			US 2003-464404P	P	20030421	<--
			WO 2004-US9272	W	20040408	

OTHER SOURCE(S): MARPAT 141:395410
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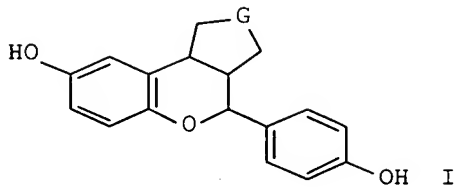

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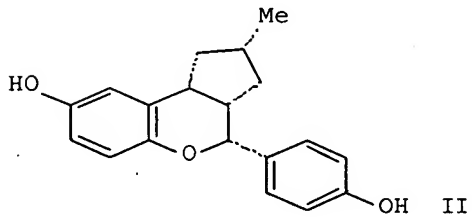


II

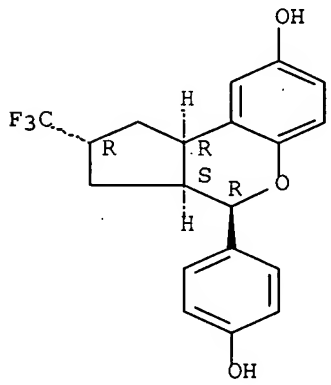
AB Title compds. represented by the formula I [wherein G = CH-alkyl, CO, CHOH, CHCF3, CF2, C(OH)CF3, CH(OH)alkyl, CH-O-alkyl, CHOCO-alkyl, etc; and their enantiomers, and pharmaceutically acceptable salts thereof] were prepared as estrogen receptor (ER)-beta agonists. For example, II was given in a multi-step synthesis starting from hydroquinone. I exhibited binding affinities (Kis) at the ER-α subtype in the range 5.0 - >10,000 nM and to the ER-β subtype in the range of 0.20 - 429 nM. Thus, I and their pharmaceutical compns. are useful as estrogen receptor agonists for the treatment of estrogen receptor mediated diseases such as prostate cancer or benign prostate hyperplasia.

IT **787621-81-2P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

RN 787621-81-2 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-(trifluoromethyl)-, (2R,3aS,4R,9bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

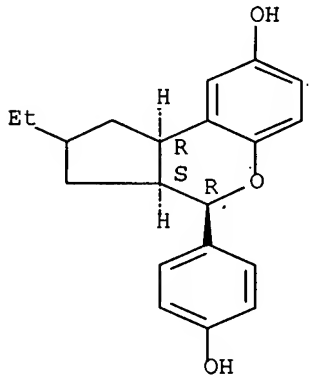


IT **787621-88-9P 787621-99-2P 787622-40-6P**
787622-43-9P 787622-78-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

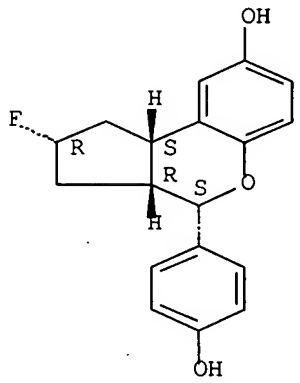
RN 787621-88-9 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 2-ethyl-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



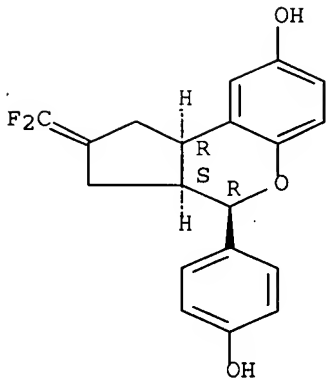
RN 787621-99-2 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 2-fluoro-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (2R,3aR,4S,9bS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



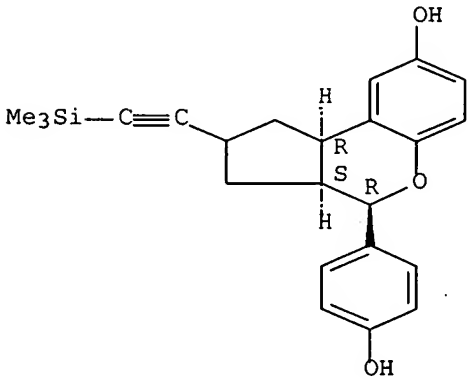
RN 787622-40-6 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 2-(difluoromethylene)-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aS,4R,9bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



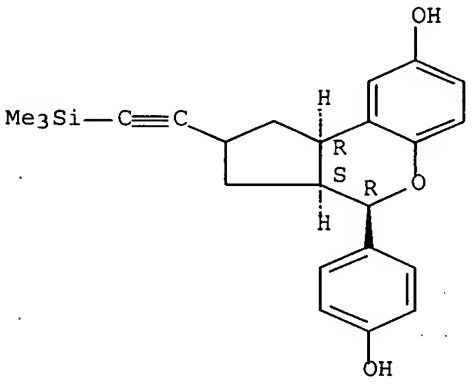
RN 787622-43-9 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-[(trimethylsilyl)ethynyl]-, (3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 787622-78-0 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-[(trimethylsilyl)ethynyl]-, (3aS,4R,9bR)- (9CI) (CA INDEX NAME)

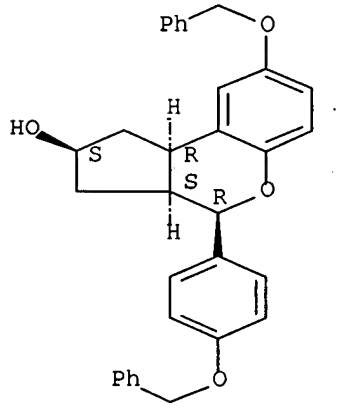
Absolute stereochemistry.



IT **787622-29-1P 787622-41-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists).

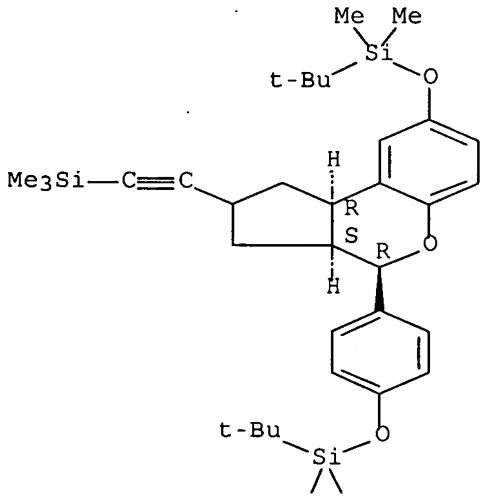
RN 787622-29-1 CAPLUS
CN Cyclopenta[c][1]benzopyran-2-ol, 1,2,3,3a,4,9b-hexahydro-8-(phenylmethoxy)-4-[4-(phenylmethoxy)phenyl]-, (2R,3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 787622-41-7 CAPLUS
CN Silane, (1,1-dimethylethyl)[4-[(3aR,4S,9bS)-8-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1,2,3,3a,4,9b-hexahydro-2-[(trimethylsilyl)ethynyl]cyclopenta[c][1]benzopyran-4-yl]phenoxy]dimethyl-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



Me Me

L5 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:417738 CAPLUS Full-text
DOCUMENT NUMBER: 139:6768
TITLE: Preparation of benzopyran derivatives as selective estrogen receptor β agonists
INVENTOR(S): Dodge, Jeffrey Alan; Krishnan, Venkatesh Gary; Lugar, Charles Willis, III; Neubauer, Blake Lee; Norman, Bryan Hurst; Pfeifer, Lance Allen; Richardson, Timothy Ivo
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 138 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003044006	A1	20030530	WO 2002-US33622	20021107 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2467013	A1	20030530	CA 2002-2467013	20021107 <--
AU 2002359283	A1	20030610	AU 2002-359283	20021107 <--
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CN 1589268	A	20050302	CN 2002-822991	20021107 <--
HU 200402628	A2	20050428	HU 2004-2628	20021107 <--
JP 2005513027	T	20050512	JP 2003-545643	20021107 <--
NZ 531850	A	20070126	NZ 2002-531850	20021107 <--
EP 1790644	A1	20070530	EP 2007-102693	20021107 <--
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AT 362471	T	20070615	AT 2002-793806	20021107 <--
US 2004249167	A1	20041209	US 2004-493092	20040420 <--
US 7217734	B2	20070515		
ZA 2004003733	A	20051004	ZA 2004-3733	20040514 <--
IN 2004KN00639	A	20060421	IN 2004-KN639	20040517 <--
MX 2004PA04703	A	20040819	MX 2004-PA4703	20040518 <--
NO 2004002583	A	20040618	NO 2004-2583	20040618 <--
PRIORITY APPLN. INFO.:			US 2001-332766P	P 20011119 <--
			US 2002-363622P	P 20020311 <--
			EP 2002-793806	A3 20021107 <--

OTHER SOURCE(S): MARPAT 139:6768

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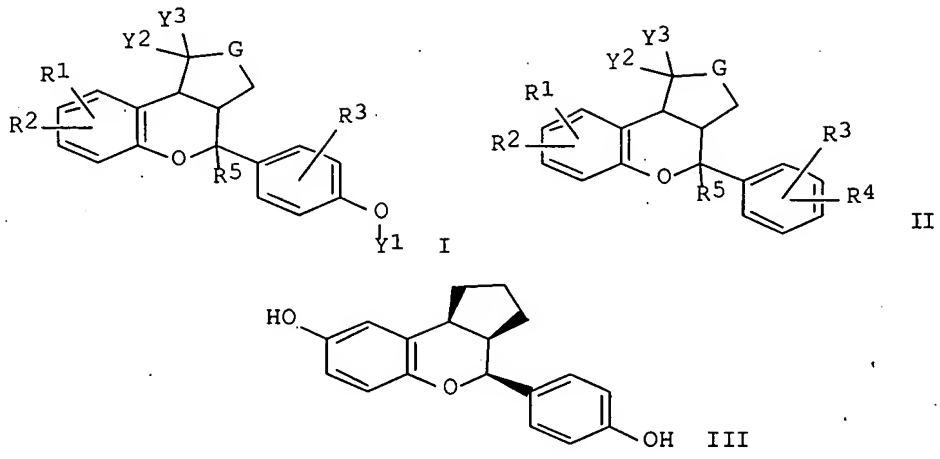


I II III

AB The title compds. I and II [wherein R1-R4 = independently H, alkyl, OH, alkoxy, halo, amido, or CF3; R5 = H or CF3; Y1-Y3 = independently H or alkyl; G = CH2, CH2CH2, or CH2CH2CH2] and stereoisomers, and pharmaceutical acceptable salts thereof are prepared as selective estrogen receptor β agonists for the treatment of prostate cancer. For example, the benzopyran III was prepared in a multi-step synthesis in moderate yield. III binds to estrogen receptor β (ER β) with a Ki of <1 nM and Ki(ER α)/Ki(ER β) of 8.0.

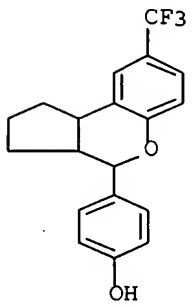
IT **533884-11-6P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of benzopyran derivs. as selective estrogen receptor β agonists)

RN 533884-11-6 CAPLUS

CN Phenol, 4-[1,2,3,3a,4,9b-hexahydro-8-(trifluoromethyl)cyclopenta[c][1]benzopyran-4-yl]- (9CI) (CA INDEX NAME)

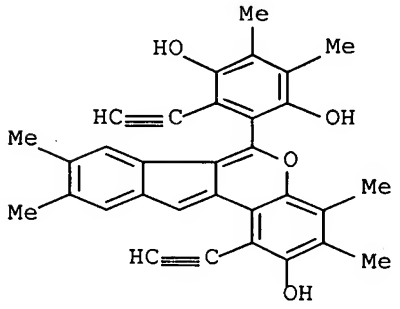


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:689997 CAPLUS Full-text
DOCUMENT NUMBER: 130:38272
TITLE: A novel tandem bicyclization to form an indenopyran ring system
AUTHOR(S): Chakraborty, Manisha; McConville, David B.; Saito, Takeshi; Meng, Huihan; Rinaldi, Peter L.; Tessier, Claire A.; Youngs, Wiley J.
CORPORATE SOURCE: Dep. of Chemistry, University of Akron, Akron, OH, 44325-3601, USA
SOURCE: Tetrahedron Letters (1998), 39(45), 8237-8340
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:38272

AB A new palladium-copper catalyzed intramol. acetylene-zipper type bicyclization between alkyne and hydroxy functionality of an alkynyl hydroquinone has been observed to give a highly conjugated ring system.

IT **216777-12-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of indenopyrans by tandem bicyclization)
RN 216777-12-7 CAPLUS
CN 1,4-Benzenediol, 2-ethynyl-3-(1-ethynyl-2-hydroxy-3,4,8,9-tetramethylbenz[b]indeno[2,1-d]pyran-6-yl)-5,6-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

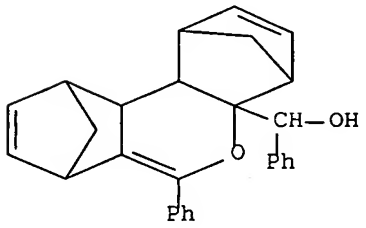
L5 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1972:152831 CAPLUS Full-text
DOCUMENT NUMBER: 76:152831
TITLE: Condensation of phenyl ethynyl ketone with cyclopentadiene. Reinvestigation
AUTHOR(S): Venkataramani, P. S.; Chandrasekharan, S.; Swaminathan, S.
CORPORATE SOURCE: Dep. Org. Chem., Univ. Madras, Madras, India
SOURCE: Tetrahedron (1972), 28(5), 1249-55
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.

AB The earlier structural assignment of 2-benzoylnorborna-diene (I) for the product obtained by the condensation of PhC-(O)C.tplbond.CH with cyclopentadiene is now revised to a dimeric structure, II.

IT **36144-49-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 36144-49-7 CAPLUS

CN 1,4:7,10-Dimethano-4aH-dibenzo[b,d]pyran-4a-methanol, 1,4,7,10,10a,10b-hexahydro-α,6-diphenyl-, [1α,4α,4aβ(R*),7β,10.beta.,10aα,10bβ]- (9CI) (CA INDEX NAME)



L5 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1969:77707 CAPLUS Full-text

DOCUMENT NUMBER: 70:77707

TITLE: Experiments in the brazilane series. I. Preparation of 2-phenyl-5',6',7-trimethoxybrazilane

AUTHOR(S): Morsingh, Francis

CORPORATE SOURCE: Univ. Malaya, Kuala Lumpur, Malay.

SOURCE: Tetrahedron (1969), 25(2), 355-9
CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

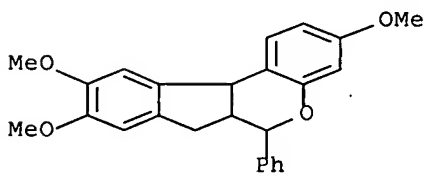
LANGUAGE: English

AB Superposition of flavan on brazilane would afford 2-phenylbrazilane. Although this structure has not yet been isolated, biogenetically it is feasible. The synthesis of 2-phenyl-5',6',7-trimethoxybrazilane is described.

IT **21834-73-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 21834-73-1 CAPLUS

CN Benz[b]indeno[1,2-d]pyran, 6,6a,7,11b-tetrahydro-3,9,10-trimethoxy-6-phenyl- (8CI) (CA INDEX NAME)



L5 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1946:23981 CAPLUS Full-text

DOCUMENT NUMBER: 40:23981

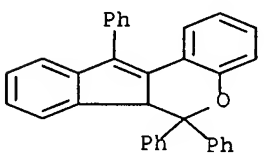
ORIGINAL REFERENCE NO.: 40:4709e-i,4710a-b
TITLE: Condensation of tetraphenylbutynediol with phenol
AUTHOR(S): Zal'kind, Yu. S.; Teterin, V. K.; Kuznetsov, S. G.
CORPORATE SOURCE: Leningrad Chem. Tech. Inst.
SOURCE: Zhurnal Obshchei Khimii (1945), 15, 488-98
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB [.tplbond.CC(OH)Ph2]2 (I) (30 g.), 87.6 g. PhOH, 60 cc. benzene and 0.4 g. dry H2NC6H4SO3H were refluxed for 2 h. with continuous removal of water by means of a Stark-Dean type collector, in which 3.35 cc. H2O was collected at the end of the reaction; after cooling and dilution with benzene, the crystalline and the liquid portions were steam-distilled to remove the solvent. There were obtained 28.7 g. crystalline matter and 16.7 g. red resin. Prolonged recrystn. from benzene, CHCl3, and ligroin gave the following products: 21.5 g. 1-diphenylmethylene-2-p-hydroxyphenyl-3-phenylindene, m. 255° (II), yellow-orange needles; 2.8 g. 1-diphenylmethylene-2- phenoxy-3-phenylindene (III), m. 223°, orange prisms; 1.2 g. 2,2,5,5-tetraphenyl-3-phenoxy-2,5-dihydrofuran, m. 176°, colorless needles; and 0.4 g. 2,2,3'-triphenyl-1',2',3,4-indenochroman (IV), m. 216-17°, colorless parallelopipeds. II was converted into the MeO derivative, m. 176-7 °, by boiling with MeI in the presence of K2CO3 in Me2CO, or by treatment with Me2SO4 in 20% NaOH; rapid crystallization from Me2CO leads to yellow needles of the above m.p., slow crystallization gives large red-brown parallelopipeds, m. 167-8°. III was prepared by an alternate method for identification: 10.5 g. I in 150 cc. Et2O was treated with 22.5 g. PCl3 at 1°over 5 h., stirred for 2 h. at 0° and for 4 h. at room temperature to yield, after removal of the solvent, hydrolysis, and crystallization from ligroin 1.0 g. 1-diphenylmethylene-2-chloro-3- phenylindene, m. 157° (cf. Wieland and Kloss, C.A. 23, 3696), and 3 unidentified products m. 147-8° (4.5 g.), m. 194-5° (0.2 g.), and m. 165° (0.4 g.); 0.4 g. of the chloride was added to a solution of 0.1 g. K in 2 g. molten PhOH and heated slowly to 220° for 1 h.; after treatment with alkaline water, extraction of the precipitate with EtOH, and crystallization of the residue from benzene-petr. ether there was obtained a product identical with III, m. 223°, above. Boiling of this in MePh in the presence of sulfanilic acid failed to effect any isomerization. IV on boiling with alc. KOH is transformed into 2 substances which were unidentified: colorless, m. 230° (from EtOH, then EtOHMe2CO), and orange, m. 208-19°, with the former transforming into a product m. 208-14°, on heating above the m.p. The condensation of I with PhOH was also conducted in the presence of the following catalysts: activated Chasoviarskii clay, H2SO4-AcOH, and glacial AcOH. The 1st catalyst gave results similar to sulfanilic acid while the 2nd catalyst gave only II, m. 255°, in 98% yield (crude); the 3rd catalyst gave only a resinous, ill-defined mixture of some transformation products of the glycol without condensation with PhOH.

IT **860186-11-4P**, Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11-triphenyl-
RL: PREP (Preparation)
(preparation of)

RN 860186-11-4 CAPLUS

CN Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11-triphenyl- (4CI) (CA INDEX NAME)



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YOU HAVE REQUESTED DATA FROM 8 ANSWERS - CONTINUE? Y/(N):y

L6   ANSWER 1 OF 8  CAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2006:381028  CAPLUS Full-text
DOCUMENT NUMBER:          144:432681
TITLE:                    Preparation of substituted benzopyrans as selective
                          estrogen receptor-beta agonists
INVENTOR(S):              Norman, Bryan Hurst; Richardson, Timothy Ivo
PATENT ASSIGNEE(S):       Eli Lilly and Company, USA
SOURCE:                   PCT Int. Appl., 50 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
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     WO 2006044176         A1    20060427    WO 2005-US35472         20051005
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
             LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ,
             NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG,
             SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN,
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         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
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             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
     CA 2578300            A1    20060427    CA 2005-2578300         20051005
     EP 1805160            A1    20070711    EP 2005-807448          20051005
         R:  AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR
PRIORITY APPLN. INFO.:                        US 2004-619627P     P  20041018
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OTHER SOURCE(S):          MARPAT 144:432681
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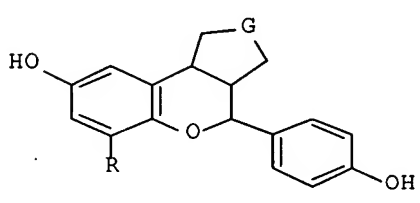

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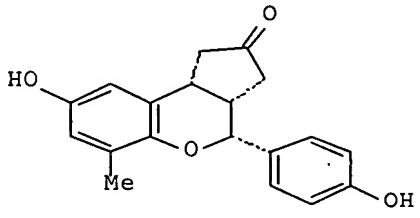


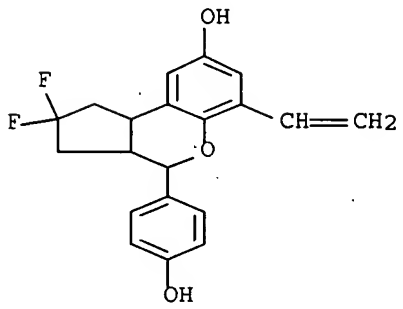
II

AB Title compds. represented by the formula I [wherein R = halo, alkyl or R3-(CH2)m; G = O, CF2, SOn, CO, CR1H or CR2(OH); R1 = F, OH, cyano, etc.; R2 = CF3 or alkyl; R3 = CN, OH, alkenyl or alkoxy(carbonyl); m = 0-2; n = 0-2; and pharmaceutical acceptable salts thereof] were prepared as estrogen receptor-beta (ER-β) agonists. For example, II was given in a multi-step synthesis starting from 3-bromo-2-hydroxy-5- methoxybenzaldehyde. I exhibited binding affinities (Kis) at the ER-α subtype in the range 4- >1000 nM and to the ER-β subtype in the range of 0.3-120 nM. Thus, I and their pharmaceutical compns. are useful as estrogen receptor agonists for the treatment of ER-β mediated diseases, such as prostate cancer or benign prostate hyperplasia (no data).

IT **885025-43-4P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted benzopyrans as selective estrogen receptor-beta agonists)

RN 885025-43-4 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 6-ethenyl-2,2-difluoro-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:369613 CAPLUS Full-text

DOCUMENT NUMBER: 144:150207

TITLE: Traceless solid-phase synthesis of cyclopenta[c]quinolines and cyclopenta[c]chromenes via hetero [6+3] cycloadditions of fulvene. A facile approach to the 11-heterosteroids framework

AUTHOR(S): Hong, Bor-Cherng; Chen, Zhong-Yi; Chen, Wei-Hung; Sun, Hsu-I.; Lee, Gene-Hsiang

CORPORATE SOURCE: Department of Chemistry and Biochemistry, National Chung Cheng University, Chia-Yi, 621, Taiwan

SOURCE: Journal of the Chinese Chemical Society (Taipei, Taiwan) (2005), 52(1), 181-200
CODEN: JCCTAC; ISSN: 0009-4536

PUBLISHER: Chinese Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:150207

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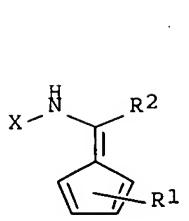

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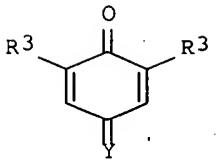

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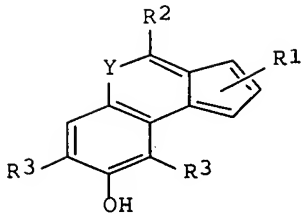


III

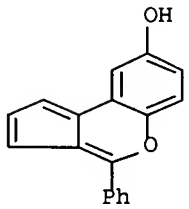
AB The hetero [6+3] cycloaddn. of resin-bound fulvenes I (X = resin; R1 = H, Me; R2 = H, Me, Et, n-Pr, n-Bu, Ph) to benzoquinones and quinonimines, e.g. II (Y = O, 4-Me2NC6H4N; R3 = H, Me, Cl), provides an efficient route to the synthesis of cyclopenta[c]chromenes and cyclopenta[c]quinolines, e.g. III. The structure of the cyclopenta[c]chromene skeleton was confirmed by the X-ray structure anal. of the 4-bromobenzoate of III (Y = O; R1 = H; R2 = R3 = Me). The antiproliferative activity of two cyclopenta[c]chromene derivs. against a number of carcinogenic human cell lines has been studied.

IT **874118-35-1P 874118-44-2P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(solution-phase and traceless solid-phase synthesis of hydroxy-substituted cyclopenta[c]quinolines and cyclopenta[c]chromenes via hetero [6+3] cycloaddns. of fulvenes with quinones or quinonimines)

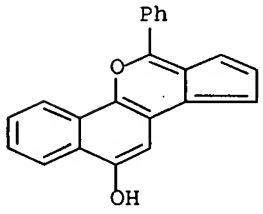
RN 874118-35-1 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 4-phenyl- (9CI) (CA INDEX NAME)



RN 874118-44-2 CAPLUS

CN Cyclopenta[d]naphtho[1,2-b]pyran-11-ol, 6-phenyl- (9CI) (CA INDEX NAME)



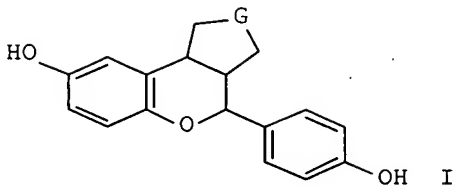
REFERENCE COUNT: 73 THERE ARE 73 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

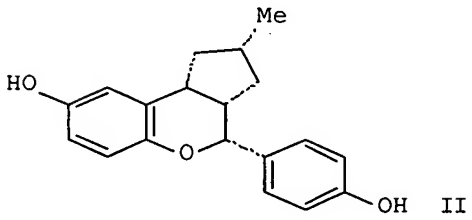
ACCESSION NUMBER: 2004:927190 CAPLUS Full-text
DOCUMENT NUMBER: 141:395410
TITLE: Preparation of substituted benzopyrans as selective estrogen receptor-beta agonists
INVENTOR(S): Durst, Gregory Lee; Norman, Bryan Hurst; Pfeifer, Lance Allen; Richardson, Timothy Ivo
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 129 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2004094400	A2	20041104	WO 2004-US9272		20040408
WO 2004094400	A3	20050224			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 2004232798	A1	20041104	AU 2004-232798		20040408
CA 2518819	A1	20041104	CA 2004-2518819		20040408
EP 1626974	A2	20060222	EP 2004-759767		20040408
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK					
BR 2004009588	A	20060418	BR 2004-9588		20040408
CN 1777614	A	20060524	CN 2004-80010817		20040408
JP 2006524240	T	20061026	JP 2006-509332		20040408
US 2007106082	A1	20070510	US 2005-552504		20051006
MX 2005PA11243	A	20051215	MX 2005-PA11243		20051019
PRIORITY APPLN. INFO.:			US 2003-464404P	P	20030421
			WO 2004-US9272	W	20040408

OTHER SOURCE(S): MARPAT 141:395410
GI



I



II

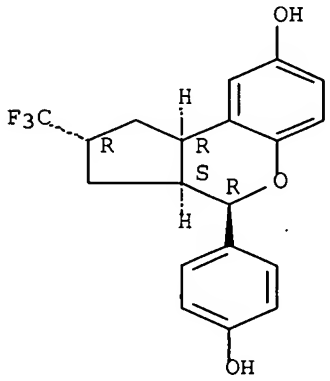
AB Title compds. represented by the formula I [wherein G = CH-alkyl, CO, CHOH, CHCF3, CF2, C(OH)CF3, CH(OH)alkyl, CH-O-alkyl, CHOCO-alkyl, etc; and their enantiomers, and pharmaceutically acceptable salts thereof] were prepared as estrogen receptor (ER)-beta agonists. For example, II was given in a multi-step synthesis starting from hydroquinone. I exhibited binding affinities (Kis) at the ER-α subtype in the range 5.0 - >10,000 nM and to the ER-β subtype in the range of 0.20 - 429 nM. Thus, I and their pharmaceutical compns. are useful as estrogen receptor agonists for the treatment of estrogen receptor mediated diseases such as prostate cancer or benign prostate hyperplasia.

IT **787621-81-2P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

RN 787621-81-2 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-(trifluoromethyl)-, (2R,3aS,4R,9bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

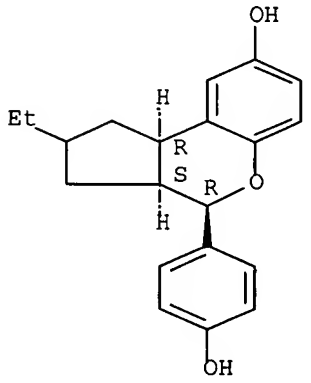


IT **787621-88-9P 787621-99-2P 787622-40-6P**
787622-43-9P 787622-78-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

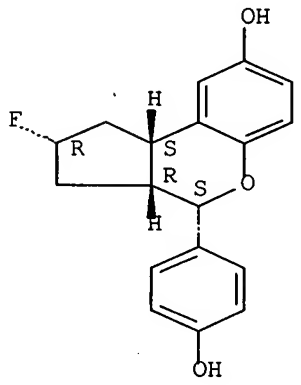
RN 787621-88-9 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 2-ethyl-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



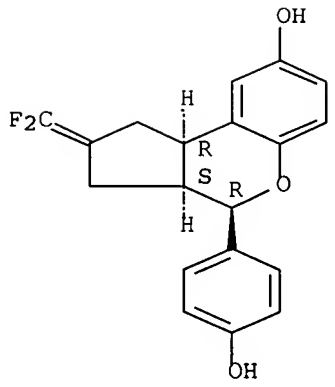
RN 787621-99-2 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 2-fluoro-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (2R,3aR,4S,9bS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



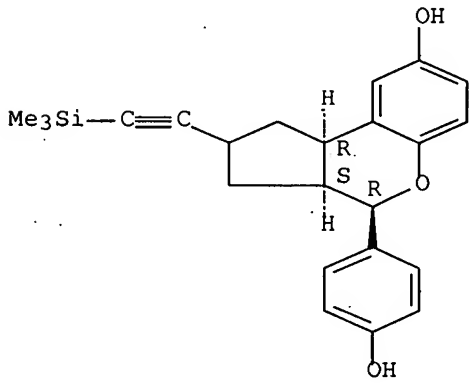
RN 787622-40-6 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 2-(difluoromethylene)-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aS,4R,9bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



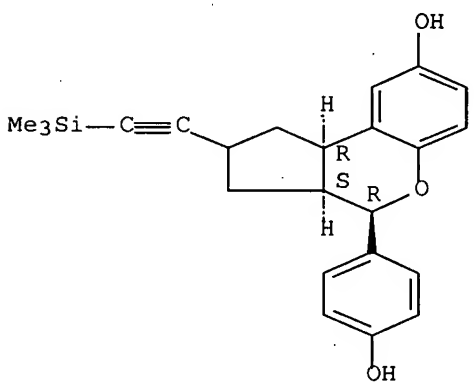
RN 787622-43-9 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-[(trimethylsilyl)ethynyl]-, (3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 787622-78-0 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-[(trimethylsilyl)ethynyl]-, (3aS,4R,9bR)- (9CI) (CA INDEX NAME)

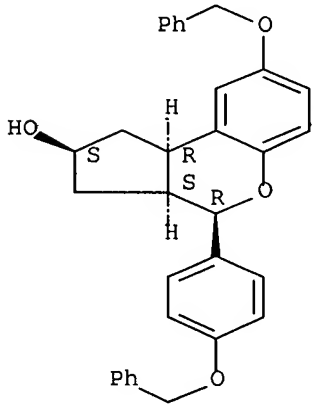
Absolute stereochemistry.



IT **787622-29-1P 787622-41-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

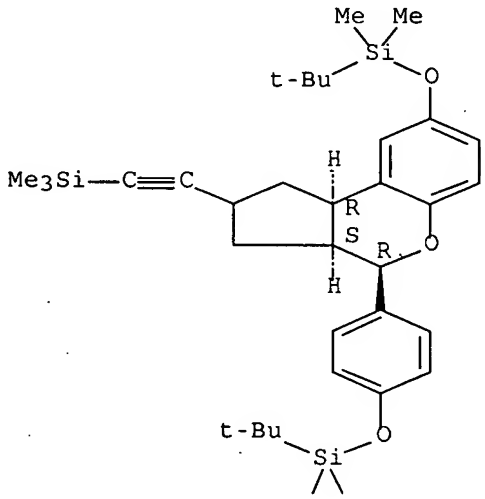
RN 787622-29-1 CAPLUS
CN Cyclopenta[c][1]benzopyran-2-ol, 1,2,3,3a,4,9b-hexahydro-8-(phenylmethoxy)-4-[4-(phenylmethoxy)phenyl]-, (2R,3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 787622-41-7 CAPLUS
CN Silane, (1,1-dimethylethyl)[4-[(3aR,4S,9bS)-8-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1,2,3,3a,4,9b-hexahydro-2-[(trimethylsilyl)ethynyl]cyclopenta[c][1]benzopyran-4-yl]phenoxy]dimethyl-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



Me Me

L6 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:417738 CAPLUS Full-text
DOCUMENT NUMBER: 139:6768
TITLE: Preparation of benzopyran derivatives as selective estrogen receptor β agonists
INVENTOR(S): Dodge, Jeffrey Alan; Krishnan, Venkatesh Gary; Lugar, Charles Willis, III; Neubauer, Blake Lee; Norman, Bryan Hurst; Pfeifer, Lance Allen; Richardson, Timothy Ivo
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 138 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003044006	A1	20030530	WO 2002-US33622	20021107
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2467013	A1	20030530	CA 2002-2467013	20021107
AU 2002359283	A1	20030610	AU 2002-359283	20021107
EP 1448544	A1	20040825	EP 2002-793806	20021107
EP 1448544	B1	20070516		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
CN 1589268	A	20050302	CN 2002-822991	20021107
HU 200402628	A2	20050428	HU 2004-2628	20021107
JP 2005513027	T	20050512	JP 2003-545643	20021107
NZ 531850	A	20070126	NZ 2002-531850	20021107
EP 1790644	A1	20070530	EP 2007-102693	20021107
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE, SK, TR, AL, LT, LV, MK, RO, SI				
AT 362471	T	20070615	AT 2002-793806	20021107
US 2004249167	A1	20041209	US 2004-493092	20040420
US 7217734	B2	20070515		
ZA 2004003733	A	20051004	ZA 2004-3733	20040514
IN 2004KN00639	A	20060421	IN 2004-KN639	20040517
MX 2004PA04703	A	20040819	MX 2004-PA4703	20040518
NO 2004002583	A	20040618	NO 2004-2583	20040618
PRIORITY APPLN. INFO.:			US 2001-332766P P	20011119
			US 2002-363622P P	20020311
			EP 2002-793806 A3	20021107

OTHER SOURCE(S): MARPAT 139:6768

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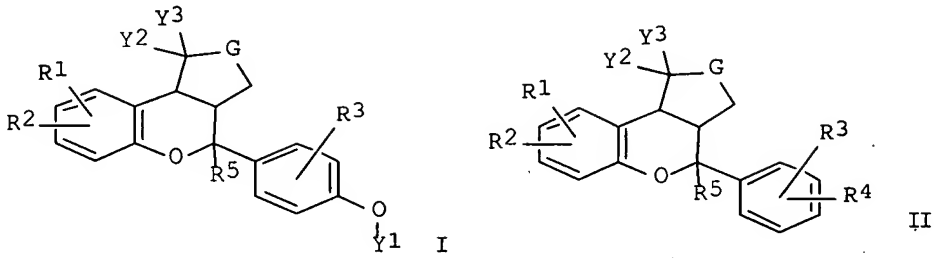
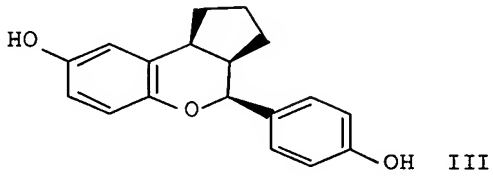




AB The title compds. I and II [wherein R1-R4 = independently H, alkyl, OH, alkoxy, halo, amido, or CF3; R5 = H or CF3; Y1-Y3 = independently H or alkyl; G = CH2, CH2CH2, or CH2CH2CH2] and stereoisomers, and pharmaceutical acceptable salts thereof are prepared as selective estrogen receptor β agonists for the treatment of prostate cancer. For example, the benzopyran III was prepared in a multi-step synthesis in moderate yield. III binds to estrogen receptor β (ER β) with a Ki of <1 nM and Ki(ER α)/Ki(ER β) of 8.0.

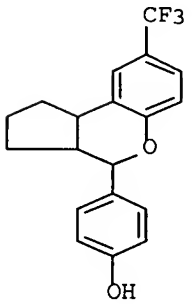
IT **533884-11-6P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of benzopyran derivs. as selective estrogen receptor β agonists)

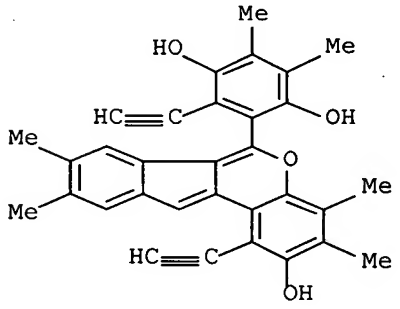
RN 533884-11-6 CAPLUS

CN Phenol, 4-[1,2,3,3a,4,9b-hexahydro-8-(trifluoromethyl)cyclopenta[c][1]benzopyran-4-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:689997 CAPLUS Full-text
DOCUMENT NUMBER: 130:38272
TITLE: A novel tandem bicyclization to form an indenopyran ring system
AUTHOR(S): Chakraborty, Manisha; McConville, David B.; Saito, Takeshi; Meng, Huihan; Rinaldi, Peter L.; Tessier, Claire A.; Youngs, Wiley J.
CORPORATE SOURCE: Dep. of Chemistry, University of Akron, Akron, OH, 44325-3601, USA
SOURCE: Tetrahedron Letters (1998), 39(45), 8237-8340
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:38272
AB A new palladium-copper catalyzed intramol. acetylene-zipper type bicyclization between alkyne and hydroxy functionality of an alkynyl hydroquinone has been observed to give a highly conjugated ring system.
IT **216777-12-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of indenopyrans by tandem bicyclization)
RN 216777-12-7 CAPLUS
CN 1,4-Benzenediol, 2-ethynyl-3-(1-ethynyl-2-hydroxy-3,4,8,9-tetramethylbenz[b]indeno[2,1-d]pyran-6-yl)-5,6-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

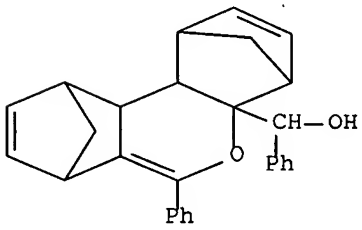
L6 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1972:152831 CAPLUS Full-text
DOCUMENT NUMBER: 76:152831
TITLE: Condensation of phenyl ethynyl ketone with cyclopentadiene. Reinvestigation
AUTHOR(S): Venkataramani, P. S.; Chandrasekharan, S.; Swaminathan, S.
CORPORATE SOURCE: Dep. Org. Chem., Univ. Madras, Madras, India
SOURCE: Tetrahedron (1972), 28(5), 1249-55
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.

AB The earlier structural assignment of 2-benzoylnorborna-diene (I) for the product obtained by the condensation of PhC-(O)C.tplbond.CH with cyclopentadiene is now revised to a dimeric structure, II.

IT **36144-49-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 36144-49-7 CAPLUS

CN 1,4:7,10-Dimethano-4aH-dibenzo[b,d]pyran-4a-methanol, 1,4,7,10,10a,10b-hexahydro-α,6-diphenyl-, [1α,4α,4aβ(R*),7β,10.beta.,10aα,10bβ]- (9CI) (CA INDEX NAME)



L6 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1969:77707 CAPLUS Full-text

DOCUMENT NUMBER: 70:77707

TITLE: Experiments in the brazilane series. I. Preparation of 2-phenyl-5',6',7-trimethoxybrazilane

AUTHOR(S): Morsingh, Francis

CORPORATE SOURCE: Univ. Malaya, Kuala Lumpur, Malay.

SOURCE: Tetrahedron (1969), 25(2), 355-9
CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

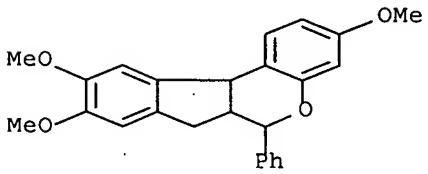
LANGUAGE: English

AB Superposition of flavan on brazilane would afford 2-phenylbrazilane. Although this structure has not yet been isolated, biogenetically it is feasible. The synthesis of 2-phenyl-5',6',7-trimethoxybrazilane is described.

IT **21834-73-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 21834-73-1 CAPLUS

CN Benz[b]indeno[1,2-d]pyran, 6,6a,7,11b-tetrahydro-3,9,10-trimethoxy-6-phenyl- (8CI) (CA INDEX NAME)



L6 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1946:23981 CAPLUS Full-text

DOCUMENT NUMBER: 40:23981

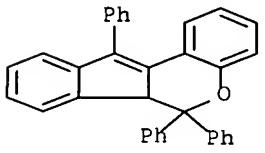
ORIGINAL REFERENCE NO.: 40:4709e-i,4710a-b
TITLE: Condensation of tetraphenylbutynediol with phenol
AUTHOR(S): Zal'kind, Yu. S.; Teterin, V. K.; Kuznetsov, S. G.
CORPORATE SOURCE: Leningrad Chem. Tech. Inst.
SOURCE: Zhurnal Obshchei Khimii (1945), 15, 488-98
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB [.tplbond.CC(OH)Ph2]2 (I) (30 g.), 87.6 g. PhOH, 60 cc. benzene and 0.4 g. dry H2NC6H4SO3H were refluxed for 2 h. with continuous removal of water by means of a Stark-Dean type collector, in which 3.35 cc. H2O was collected at the end of the reaction; after cooling and dilution with benzene, the crystalline and the liquid portions were steam-distilled to remove the solvent. There were obtained 28.7 g. crystalline matter and 16.7 g. red resin. Prolonged recrystn. from benzene, CHCl3, and ligroin gave the following products: 21.5 g. 1-diphenylmethylene-2-p-hydroxyphenyl-3-phenylindene, m. 255° (II), yellow-orange needles; 2.8 g. 1-diphenylmethylene-2- phenoxy-3-phenylindene (III), m. 223°, orange prisms; 1.2 g. 2,2,5,5-tetraphenyl-3-phenoxy-2,5-dihydrofuran, m. 176°, colorless needles; and 0.4 g. 2,2,3'-triphenyl-1',2',3,4-indenochroman (IV), m. 216-17°, colorless parallelopipeds. II was converted into the MeO derivative, m. 176-7 °, by boiling with MeI in the presence of K2CO3 in Me2CO, or by treatment with Me2SO4 in 20% NaOH; rapid crystallization from Me2CO leads to yellow needles of the above m.p., slow crystallization gives large red-brown parallelopipeds, m. 167-8°. III was prepared by an alternate method for identification: 10.5 g. I in 150 cc. Et2O was treated with 22.5 g. PCl3 at 1°over 5 h., stirred for 2 h. at 0° and for 4 h. at room temperature to yield, after removal of the solvent, hydrolysis, and crystallization from ligroin 1.0 g. 1-diphenylmethylene-2-chloro-3- phenylindene, m. 157° (cf. Wieland and Kloss, C.A. 23, 3696), and 3 unidentified products m. 147-8° (4.5 g.), m. 194-5° (0.2 g.), and m. 165° (0.4 g.); 0.4 g. of the chloride was added to a solution of 0.1 g. K in 2 g. molten PhOH and heated slowly to 220° for 1 h.; after treatment with alkaline water, extraction of the precipitate with EtOH, and crystallization of the residue from benzene-petr. ether there was obtained a product identical with III, m. 223°, above. Boiling of this in MePh in the presence of sulfanilic acid failed to effect any isomerization. IV on boiling with alc. KOH is transformed into 2 substances which were unidentified: colorless, m. 230° (from EtOH, then EtOHMe2CO), and orange, m. 208-19°, with the former transforming into a product m. 208-14°, on heating above the m.p. The condensation of I with PhOH was also conducted in the presence of the following catalysts: activated Chasoviarskii clay, H2SO4-AcOH, and glacial AcOH. The 1st catalyst gave results similar to sulfanilic acid while the 2nd catalyst gave only II, m. 255°, in 98% yield (crude); the 3rd catalyst gave only a resinous, ill-defined mixture of some transformation products of the glycol without condensation with PhOH.

IT **860186-11-4P**, Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11-triphenyl-
RL: PREP (Preparation)
(preparation of)

RN 860186-11-4 CAPLUS

CN Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11-triphenyl- (4CI) (CA INDEX NAME)



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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   101.43     115.59

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                   -10.92     -10.92

FILE 'REGISTRY' ENTERED AT 15:12:49 ON 06 AUG 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:     5 AUG 2007  HIGHEST RN 944042-79-9
DICTIONARY FILE UPDATES:    5 AUG 2007  HIGHEST RN 944042-79-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10-552504b.str


L7      STRUCTURE UPLOADED

=> d l7
L7 HAS NO ANSWERS
L7              STR
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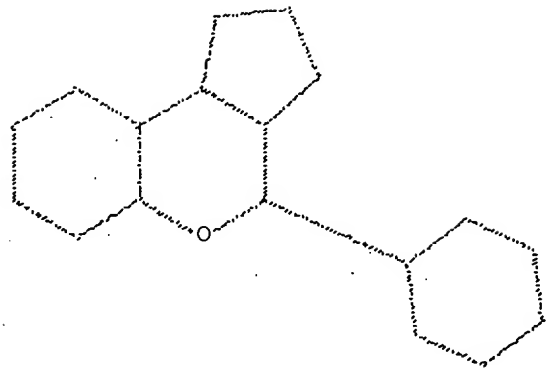

Structure attributes must be viewed using STN Express query preparation.

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=> s l7 sss sam
SAMPLE SEARCH INITIATED 15:13:58 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     1636 TO ITERATE

100.0% PROCESSED     1636 ITERATIONS                                 17 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        30294 TO    35146
PROJECTED ANSWERS:              93 TO      587

L8            17 SEA SSS SAM L7

=> d scan

L8   17 ANSWERS   REGISTRY  COPYRIGHT 2007 ACS on STN
IN   Cyclopenta[c][1]benzopyran-8-ol, 4-phenyl- (9CI)
MF   C18 H12 O2
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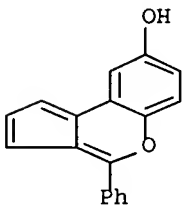

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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L8   17 ANSWERS   REGISTRY  COPYRIGHT 2007 ACS on STN
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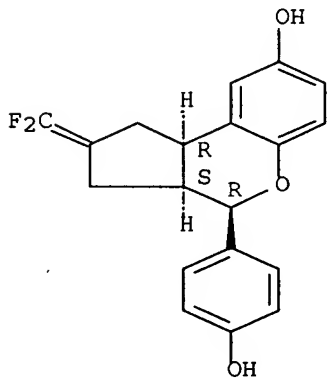
IN Cyclopenta[c][1]benzopyran-8-ol, 2-(difluoromethylene)-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aS,4R,9bR)- (9CI)
MF C19 H16 F2 O3

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

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FULL SCREEN SEARCH COMPLETED - 31330 TO ITERATE

100.0% PROCESSED 31330 ITERATIONS 281 ANSWERS
SEARCH TIME: 00.00.01

L9 281 SEA SSS FUL L7

=> s l7 and (py<2004 or ay<2004 or pry<2004)
COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID
The query entered contains both search terms created by structure-building or screen commands and text search terms. L#s created via the STRUCTURE or SCREEN commands must be searched in the structures files separately from text terms or profiles. The L# answer sets from structure searches can be used in crossover searches and can be combined with text terms.

=> s l9 and (py<2004 or ay<2004 or pry<2004)
'2004' NOT A VALID FIELD CODE
'2004' NOT A VALID FIELD CODE
'2004' NOT A VALID FIELD CODE
0 PY<2004
0 AY<2004
0 PRY<2004
L10 0 L9 AND (PY<2004 OR AY<2004 OR PRY<2004)

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION

FULL ESTIMATED COST 175.25 290.84

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY TOTAL SESSION

CA SUBSCRIBER PRICE 0.00 -10.92

FILE 'CAPLUS' ENTERED AT 15:17:21 ON 06 AUG 2007
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FILE COVERS 1907 - 6 Aug 2007 VOL 147 ISS 7
FILE LAST UPDATED: 5 Aug 2007 (20070805/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l7 and (py<2004 or ay<2004 or pry<2004)
REGISTRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 15:17:34 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1636 TO ITERATE

100.0% PROCESSED 1636 ITERATIONS 17 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 30294 TO 35146
PROJECTED ANSWERS: 93 TO 587

L11 17 SEA SSS SAM L7

L12 8 L11

23927525 PY<2004
4731037 AY<2004
4212934 PRY<2004

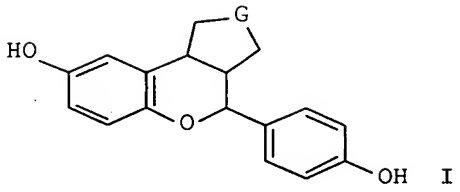
L13 6 L12 AND (PY<2004 OR AY<2004 OR PRY<2004)

=> d ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 6 ANSWERS - CONTINUE? Y/(N):y

L13 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:927190 CAPLUS Full-text
DOCUMENT NUMBER: 141:395410
TITLE: Preparation of substituted benzopyrans as selective estrogen receptor-beta agonists
INVENTOR(S): Durst, Gregory Lee; Norman, Bryan Hurst; Pfeifer, Lance Allen; Richardson, Timothy Ivo
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 129 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2004094400	A2	20041104	WO 2004-US9272		20040408 <--
WO 2004094400	A3	20050224			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 2004232798	A1	20041104	AU 2004-232798		20040408 <--
CA 2518819	A1	20041104	CA 2004-2518819		20040408 <--
EP 1626974	A2	20060222	EP 2004-759767		20040408 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK					
BR 2004009588	A	20060418	BR 2004-9588		20040408 <--
CN 1777614	A	20060524	CN 2004-80010817		20040408 <--
JP 2006524240	T	20061026	JP 2006-509332		20040408 <--
US 2007106082	A1	20070510	US 2005-552504		20051006 <--
MX 2005PA11243	A	20051215	MX 2005-PA11243		20051019 <--
PRIORITY APPLN. INFO.:			US 2003-464404P	P	20030421 <--
			WO 2004-US9272	W	20040408

OTHER SOURCE(S): MARPAT 141:395410
GI



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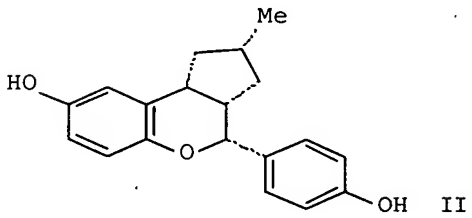


II

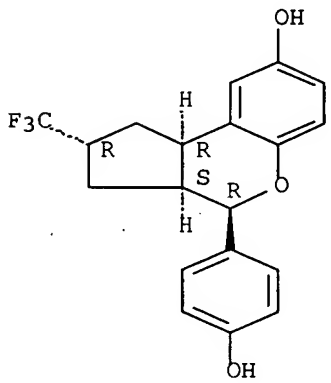
AB Title compds. represented by the formula I [wherein G = CH-alkyl, CO, CHOH, CHCF3, CF2, C(OH)CF3, CH(OH)alkyl, CH-O-alkyl, CHOCO-alkyl, etc; and their enantiomers, and pharmaceutically acceptable salts thereof] were prepared as estrogen receptor (ER)-beta agonists. For example, II was given in a multi-step synthesis starting from hydroquinone. I exhibited binding affinities (Kis) at the ER-α subtype in the range 5.0 - >10,000 nM and to the ER-β subtype in the range of 0.20 - 429 nM. Thus, I and their pharmaceutical compns. are useful as estrogen receptor agonists for the treatment of estrogen receptor mediated diseases such as prostate cancer or benign prostate hyperplasia.

IT **787621-81-2P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

RN 787621-81-2 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-(trifluoromethyl)-, (2R,3aS,4R,9bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

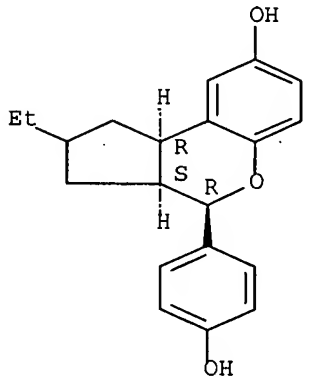


IT **787621-88-9P 787621-99-2P 787622-40-6P**
787622-43-9P 787622-78-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

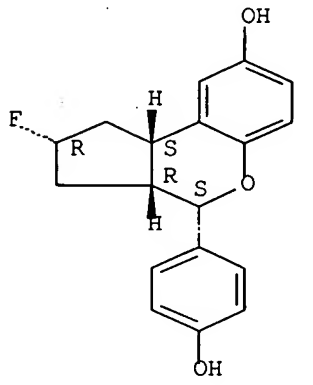
RN 787621-88-9 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 2-ethyl-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



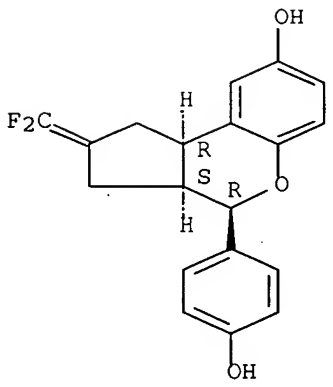
RN 787621-99-2 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 2-fluoro-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (2R,3aR,4S,9bS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



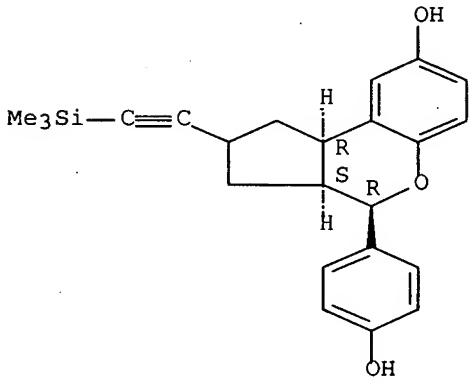
RN 787622-40-6 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 2-(difluoromethylene)-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aS,4R,9bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



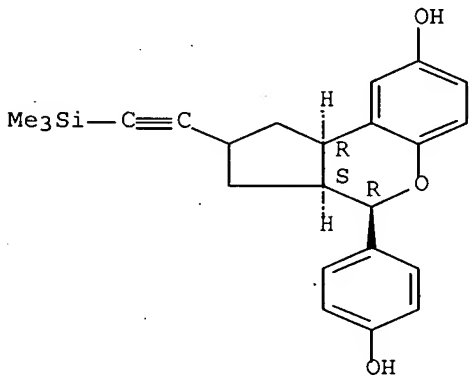
RN 787622-43-9 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-[(trimethylsilyl)ethynyl]-, (3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 787622-78-0 CAPLUS
CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-[(trimethylsilyl)ethynyl]-, (3aS,4R,9bR)- (9CI) (CA INDEX NAME)

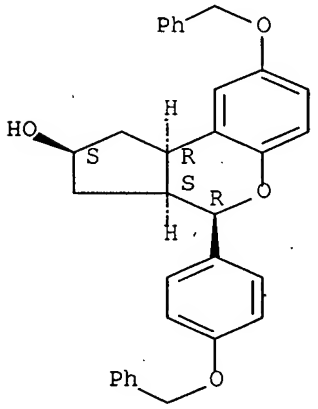
Absolute stereochemistry.



IT 787622-29-1P 787622-41-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

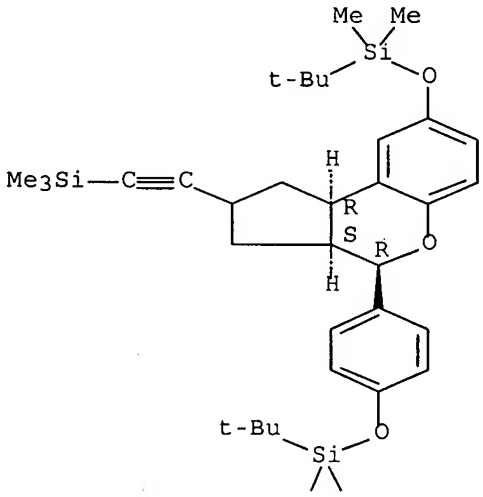
RN 787622-29-1 CAPLUS
CN Cyclopenta[c][1]benzopyran-2-ol, 1,2,3,3a,4,9b-hexahydro-8-(phenylmethoxy)-4-[4-(phenylmethoxy)phenyl]-, (2R,3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 787622-41-7 CAPLUS
CN Silane, (1,1-dimethylethyl)[4-[(3aR,4S,9bS)-8-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1,2,3,3a,4,9b-hexahydro-2-[(trimethylsilyl)ethynyl]cyclopenta[c][1]benzopyran-4-yl]phenoxy]dimethyl-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



Me Me

L13 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:417738 CAPLUS Full-text
DOCUMENT NUMBER: 139:6768
TITLE: Preparation of benzopyran derivatives as selective estrogen receptor β agonists
INVENTOR(S): Dodge, Jeffrey Alan; Krishnan, Venkatesh Gary; Lugar, Charles Willis, III; Neubauer, Blake Lee; Norman, Bryan Hurst; Pfeifer, Lance Allen; Richardson, Timothy Ivo
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 138 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2003044006	A1	20030530	WO 2002-US33622		20021107 <--
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2467013	A1	20030530	CA 2002-2467013		20021107 <--
AU 2002359283	A1	20030610	AU 2002-359283		20021107 <--
EP 1448544	A1	20040825	EP 2002-793806		20021107 <--
EP 1448544	B1	20070516			
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CN 1589268	A	20050302	CN 2002-822991		20021107 <--
HU 200402628	A2	20050428	HU 2004-2628		20021107 <--
JP 2005513027	T	20050512	JP 2003-545643		20021107 <--
NZ 531850	A	20070126	NZ 2002-531850		20021107 <--
EP 1790644	A1	20070530	EP 2007-102693		20021107 <--
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AT 362471	T	20070615	AT 2002-793806		20021107 <--
US 2004249167	A1	20041209	US 2004-493092		20040420 <--
US 7217734	B2	20070515			
ZA 2004003733	A	20051004	ZA 2004-3733		20040514 <--
IN 2004KN00639	A	20060421	IN 2004-KN639		20040517 <--
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NO 2004002583	A	20040618	NO 2004-2583		20040618 <--
PRIORITY APPLN. INFO.:			US 2001-332766P	P	20011119 <--
			US 2002-363622P	P	20020311 <--
			EP 2002-793806	A3	20021107 <--

WO 2002-US33622 W 20021107 <--

OTHER SOURCE(S): MARPAT 139:6768

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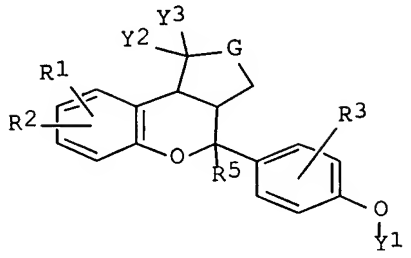

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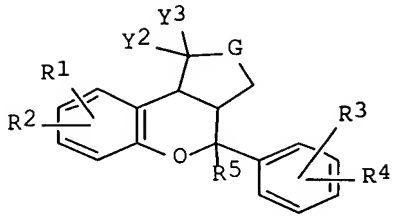
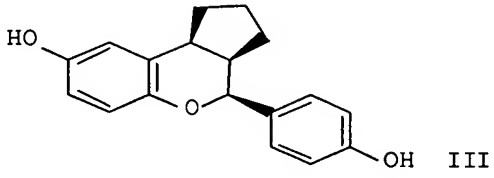


II



III

AB The title compds. I and II [wherein R1-R4 = independently H, alkyl, OH, alkoxy, halo, amido, or CF3; R5 = H or CF3; Y1-Y3 = independently H or alkyl; G = CH2, CH2CH2, or CH2CH2CH2] and stereoisomers, and pharmaceutical acceptable salts thereof are prepared as selective estrogen receptor β agonists for the treatment of prostate cancer. For example, the benzopyran III was prepared in a multi-step synthesis in moderate yield. III binds to estrogen receptor β (ER β) with a Ki of <1 nM and Ki(ER α)/Ki(ER β) of 8.0.

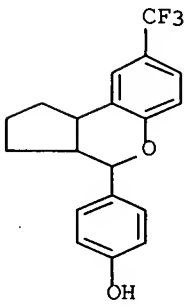
IT **533884-11-6P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of benzopyran derivs. as selective estrogen receptor β agonists)

RN 533884-11-6 CAPLUS

CN Phenol, 4-[1,2,3,3a,4,9b-hexahydro-8-(trifluoromethyl)cyclopenta[c][1]benzopyran-4-yl]- (9CI) (CA INDEX NAME)



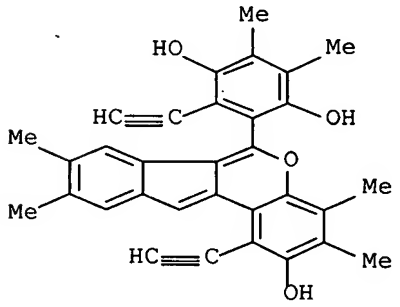
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:689997 CAPLUS Full-text
DOCUMENT NUMBER: 130:38272
TITLE: A novel tandem bicyclization to form an indenopyran ring system
AUTHOR(S): Chakraborty, Manisha; McConville, David B.; Saito, Takeshi; Meng, Huihan; Rinaldi, Peter L.; Tessier, Claire A.; Youngs, Wiley J.
CORPORATE SOURCE: Dep. of Chemistry, University of Akron, Akron, OH, 44325-3601, USA
SOURCE: Tetrahedron Letters (1998), 39(45), 8237-8340
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:38272

AB A new palladium-copper catalyzed intramol. acetylene-zipper type bicyclization between alkyne and hydroxy functionality of an alkynyl hydroquinone has been observed to give a highly conjugated ring system.

IT **216777-12-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of indenopyrans by tandem bicyclization)

RN 216777-12-7 CAPLUS
CN 1,4-Benzenediol, 2-ethynyl-3-(1-ethynyl-2-hydroxy-3,4,8,9-tetramethylbenz[b]indeno[2,1-d]pyran-6-yl)-5,6-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

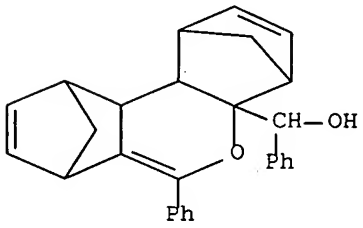
L13 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1972:152831 CAPLUS Full-text
DOCUMENT NUMBER: 76:152831
TITLE: Condensation of phenyl ethynyl ketone with cyclopentadiene. Reinvestigation
AUTHOR(S): Venkataramani, P. S.; Chandrasekharan, S.; Swaminathan, S.
CORPORATE SOURCE: Dep. Org. Chem., Univ. Madras, Madras, India
SOURCE: Tetrahedron (1972), 28(5), 1249-55
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.

AB The earlier structural assignment of 2-benzoylnorborna-diene (I) for the product obtained by the condensation of PhC-(O)C.tplbond.CH with cyclopentadiene is now revised to a dimeric structure, II.

IT **36144-49-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 36144-49-7 CAPLUS

CN 1,4:7,10-Dimethano-4aH-dibenzo[b,d]pyran-4a-methanol, 1,4,7,10,10a,10b-hexahydro-α,6-diphenyl-, [1α,4α,4aβ(R*),7β,10.beta.,10aα,10bβ]- (9CI) (CA INDEX NAME)



L13 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1969:77707 CAPLUS Full-text

DOCUMENT NUMBER: 70:77707

TITLE: Experiments in the brazilane series. I. Preparation of 2-phenyl-5',6',7-trimethoxybrazilane

AUTHOR(S): Morsingh, Francis

CORPORATE SOURCE: Univ. Malaya, Kuala Lumpur, Malay.

SOURCE: Tetrahedron (1969), 25(2), 355-9
CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

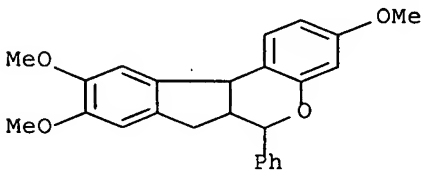
LANGUAGE: English

AB Superposition of flavan on brazilane would afford 2-phenylbrazilane. Although this structure has not yet been isolated, biogenetically it is feasible. The synthesis of 2-phenyl-5',6',7-trimethoxybrazilane is described.

IT **21834-73-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 21834-73-1 CAPLUS

CN Benz[b]indeno[1,2-d]pyran, 6,6a,7,11b-tetrahydro-3,9,10-trimethoxy-6-phenyl- (8CI) (CA INDEX NAME)



L13 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1946:23981 CAPLUS Full-text

DOCUMENT NUMBER: 40:23981

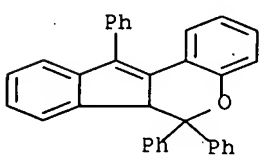
ORIGINAL REFERENCE NO.: 40:4709e-i,4710a-b
TITLE: Condensation of tetraphenylbutynediol with phenol
AUTHOR(S): Zal'kind, Yu. S.; Teterin, V. K.; Kuznetsov, S. G.
CORPORATE SOURCE: Leningrad Chem. Tech. Inst.
SOURCE: Zhurnal Obshchei Khimii (1945), 15, 488-98
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB [.tplbond.CC(OH)Ph2]2 (I) (30 g.), 87.6 g. PhOH, 60 cc. benzene and 0.4 g. dry H2NC6H4SO3H were refluxed for 2 h. with continuous removal of water by means of a Stark-Dean type collector, in which 3.35 cc. H2O was collected at the end of the reaction; after cooling and dilution with benzene, the crystalline and the liquid portions were steam-distilled to remove the solvent. There were obtained 28.7 g. crystalline matter and 16.7 g. red resin. Prolonged recrystn. from benzene, CHCl3, and ligroin gave the following products: 21.5 g. 1-diphenylmethylene-2-p-hydroxyphenyl-3-phenylindene, m. 255° (II), yellow-orange needles; 2.8 g. 1-diphenylmethylene-2- phenoxy-3-phenylindene (III), m. 223°, orange prisms; 1.2 g. 2,2,5,5-tetraphenyl-3-phenoxy-2,5-dihydrofuran, m. 176°, colorless needles; and 0.4 g. 2,2,3'-triphenyl-1',2',3,4-indenochroman (IV), m. 216-17°, colorless parallelopipeds. II was converted into the MeO derivative, m. 176-7 °, by boiling with MeI in the presence of K2CO3 in Me2CO, or by treatment with Me2SO4 in 20% NaOH; rapid crystallization from Me2CO leads to yellow needles of the above m.p., slow crystallization gives large red-brown parallelopipeds, m. 167-8°. III was prepared by an alternate method for identification: 10.5 g. I in 150 cc. Et2O was treated with 22.5 g. PCl3 at 1°over 5 h., stirred for 2 h. at 0° and for 4 h. at room temperature to yield, after removal of the solvent, hydrolysis, and crystallization from ligroin 1.0 g. 1-diphenylmethylene-2-chloro-3- phenylindene, m. 157° (cf. Wieland and Kloss, C.A. 23, 3696), and 3 unidentified products m. 147-8° (4.5 g.), m. 194-5° (0.2 g.), and m. 165° (0.4 g.); 0.4 g. of the chloride was added to a solution of 0.1 g. K in 2 g. molten PhOH and heated slowly to 220° for 1 h.; after treatment with alkaline water, extraction of the precipitate with EtOH, and crystallization of the residue from benzene-petr. ether there was obtained a product identical with III, m. 223°, above. Boiling of this in MePh in the presence of sulfanilic acid failed to effect any isomerization. IV on boiling with alc. KOH is transformed into 2 substances which were unidentified: colorless, m. 230° (from EtOH, then EtOHMe2CO), and orange, m. 208-19°, with the former transforming into a product m. 208-14°, on heating above the m.p. The condensation of I with PhOH was also conducted in the presence of the following catalysts: activated Chasoviarskii clay, H2SO4-AcOH, and glacial AcOH. The 1st catalyst gave results similar to sulfanilic acid while the 2nd catalyst gave only II, m. 255°, in 98% yield (crude); the 3rd catalyst gave only a resinous, ill-defined mixture of some transformation products of the glycol without condensation with PhOH.

IT **860186-11-4P**, Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11-triphenyl-
RL: PREP (Preparation)
(preparation of)

RN 860186-11-4 CAPLUS

CN Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11-triphenyl- (4CI) (CA INDEX NAME)



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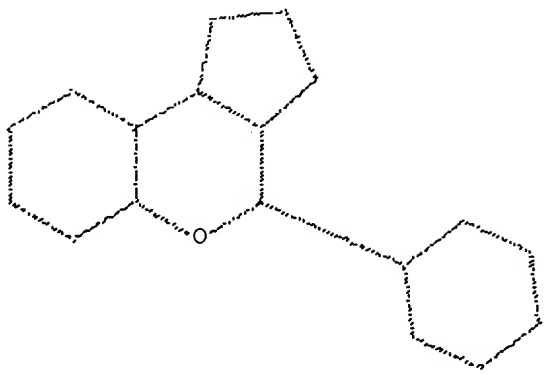

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